Singularités dans le modèle de Landau-de Gennes pour les cristaux liquides

Giacomo Canevari

Université Pierre et Marie Curie – Paris 6 **UFR 929 – Mathématiques**

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THÈSE

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par

Giacomo CANEVARI

Composition du jury

Rapporteurs :	Radu IGNAT Arghir D. ZARNESCU
Examinateurs :	John M. BALL Vincent MILLOT Petru MIRONESCU Didier SMETS
Directeur de thèse :	Fabrice BETHUEL

Laboratoire Jacques-Louis Lions — UMR 7598

"... perché il sapere germoglia"

Si j'ai pu mener cette thèse à son terme, c'est grâce à l'aide de nombreuses personnes, qui n'ont jamais manqué de me soutenir tout au long de ces trois ans. Laissez-moi profiter de ce moment pour leur dire ma gratitude, mon estime, mon affection.

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Introduction générale

Introduction générale

Dans cette thèse, nous nous intéressons principalement à l'étude de la fonctionnelle de Landau-de Gennes

$$E_\varepsilon(Q) := \int_\Omega \left\{ \frac{1}{2} |\nabla Q|^2 + \frac{1}{\varepsilon^2} f(Q) \right\},$$

où Ω est un domaine borné et régulier dans $\mathbb{R}^N$ avec $N \in \{2, 3\}$, la fonction Q prend ses valeurs dans l'espace $\mathbf{S}_0$ des matrices 3×3 réelles, symétriques et à trace nulle, et le potentiel f est donné par

$$f(Q) := k_0 - \frac{a}{2} \operatorname{tr} Q^2 - \frac{b}{3} \operatorname{tr} Q^3 + \frac{c}{4} \left(\operatorname{tr} Q^2\right)^2$$

(a, b et c sont des constantes strictement positives). Cette fonctionnelle représente un modèle simplifié pour l'énergie d'une distribution de cristaux liquides nématiques. Nous nous attacherons à l'étude de certaines propriétés des minimiseurs ainsi qu'à leur analyse asymptotique lorsque la constante élastique ε^2 tend vers 0.

Ce chapitre introductif décrit l'origine physique du modèle, en faisant un parallèle avec d'autres modèles fréquemment utilisés pour les cristaux liquides, et présente les contributions apportées par cette thèse. Le chapitre est organisé de la façon suivante. Dans la section 0.1 nous rappelons des propriétés physiques de base des cristaux liquides nématiques, en portant une attention particulière à la théorie homotopique des défauts qui caractérisent ces matériaux. La section 0.2 décrit rapidement deux modèles variationnels pour les cristaux liquides — celui d'Oseen-Frank et celui d'Ericksen — qui sont en rapport avec la théorie de Landau-de Gennes. Cette dernière fait l'objet de la section 0.3, qui traite son interprétation physique ainsi que certains problèmes mathématiques auxquels nous nous intéresserons par la suite. Les contributions apportées par cette thèse sont présentées dans les sections 0.4, 0.5 et 0.6, consacrées respectivement à l'étude qualitatif des minimiseurs, à leur analyse asymptotique et à l'étude d'un cas particulier, où le domaine est une couronne dans $\mathbb{R}^3$. La section 0.7 porte sur un sujet différent, à savoir la topologie des champs de vecteurs de faible régularité. Les résultats qui y sont contenus sont motivés par des questions d'analyse des modèles variationnels pour les cristaux liquides nématiques étalés sur une surface. Enfin, une discussion sur les possibles directions futures de recherche conclut le chapitre.

Notations

Nous introduisons ici quelques notations qui seront utilisées tout au long de cette thèse.

◇ La boule euclidienne *ouverte* de $\mathbb{R}^k$, de centre x et rayon r, sera dénotée indifféremment par $B^k_r(x)$ ou $B^k(x, r)$. Nous omettrons d'indiquer le centre si $x = 0$. Dans le cas $k = 3$, on écrira simplement $B_r(x)$, $B(x, r)$ ou encore B_r (lorsque $x = 0$). Pour les boules *fermés*, on utilisera la notation $\overline{B}_r(x)$ ou $\overline{B}(x, r)$. Les boules ouvertes dans un espace métrique X autre que $\mathbb{R}^k$ seront dénotées $B^X_r(x)$ ou $B^X(x, r)$.

◇ Le produit scalaire entre deux vecteurs $\mathbf{u}$, $\mathbf{v} \in \mathbb{R}^3$ sera noté $\mathbf{u} \cdot \mathbf{v}$, le produit vectoriel $\mathbf{u} \times \mathbf{v}$. Le symbole $\perp$ désigne l'orthogonalité ou bien entre deux vecteurs ou bien entre un vecteur et un sous-espace linéaire.

◇ Nous noterons $\mathrm{M}_3(\mathbb{R})$ l'espace des matrices réelles 3×3.

◇ Pour tout $\mathbf{p} \in \mathbb{R}^3$, on notera $\mathbf{p}^{\otimes 2}$ la matrice telle que $(\mathbf{p}^{\otimes 2})_{ij} := p_i p_j$, pour $i, j \in \{1, 2, 3\}$.

◇ Nous utiliserons ∇ pour dénoter le gradient par rapport à la variable $x \in \mathbb{R}^N$, et D pour la différentielle par rapport à $Q \in \mathbf{S}_0$. Puisque l'espace $\mathbf{S}_0$ est muni d'un produit scalaire qu'on précisera ensuite, nous identifierons canoniquement D avec un gradient. Nous noterons $\nabla_\top$ l'opérateur de dérivation dans les directions tangentes à $\partial\Omega \subset \mathbb{R}^N$.

◇ Pour toute variété $\mathscr{N}$ et tout $p \in \mathscr{N}$, l'espace tangent à $\mathscr{N}$ au point p sera noté $T_p\mathscr{N}$.

◇ Étant donné un ensemble borélien $A \subset \mathbb{R}^N$, de dimension de Hausdorff k, on notera

$$E_\varepsilon(Q, A) := \int_A \left\{ \frac{1}{2} |\nabla Q|^2 + \frac{1}{\varepsilon^2} f(Q) \right\} \mathrm{d}\mathscr{H}^k.$$

Nous omettrons d'indiquer la mesure $\mathrm{d}\mathscr{H}^3$ dans les intégrales.

1 Les cristaux liquides nématiques

1.1 Nomenclature et classification

Les cristaux liquides sont des états de la matière qui possèdent simultanément des propriétés d'un liquide et celles d'un solide cristallisé. Comme les liquides, ils sont fluides, peuvent former des gouttelettes qui s'unissent par coalescence, et ne supportent pas le cisaillement. D'autre part, ils présentent des anisotropies par rapport à certaines propriétés optiques, électriques ou magnétiques, qui sont caractéristiques d'une structure moléculaire ordonnée. Ces états de la matière — appelés plus précisément *états mésomorphes* ou *mésophases* — apparaissent car, pour une certaine classe de substances organiques dites *mésogènes*, la transition de phase liquide-solide ne se fait pas en une étape, mais procède à travers une ou plusieurs transitions intermédiaires.

Le concept des cristaux liquides fut introduit par le physicien allemand Lehmann en 1889 [84]. Le point de départ pour les études de Lehmann furent des observations conduites précédemment par des biologistes, en particulier par le botaniste autrichien Reinitzer. Dans les années suivantes, beaucoup d'autres observations furent conduites. Néanmoins, ce ne fut qu'en 1922 que Friedel, un cristallographe français, mit en évidence la nature du phénomène. Friedel remarqua [49] que les cristaux liquides constituaient une phase intermédiaire de la matière entre les états solides et liquides, et proposa la nomenclature utilisée encore aujourd'hui.

Les mésophases se classifient suivant les paramètres physiques qui induit le changement de phase. Dans les mésophases *thermotropes*, le changement de phase est fonction de la température. Par contre, dans les phases *lyotropes* le changement de phase se produit en présence d'un solvant, et dépend de la concentration du mésogène ainsi que de la température. Parmi les phases thermotropes, une classification ultérieure a été mise en place, en fonction du type d'auto-organisation des molécules. Typiquement, nous pouvons considérer au moins deux classes de mésophases thermotropes : les *nématiques* et les *smectiques* (voir la figure 1). Dans les nématiques, la distribution des centres de gravité des molécules est aléatoire, mais les molécules demeurent en moyenne parallèles les unes aux autres. Dans ce cas, il existe un ordre d'orientation à longue portée, mais pas d'ordre selon la position. Ces phases sont les moins organisées,

FIGURE 1 – Représentation schématique des mésophases. De gauche vers droite : phase nématique, cholestérique, smectique. La phase smectique comprend deux sous-phases, selon l'orientation des molécules qui peut être orthogonale au plan des couches (smectique A) ou pas (smectique C). Images réalisées par Kebes (travail personnel), [GFDL, CC BY-SA 3.0], via Wikimedia Commons.

et donc les plus proches du liquide ordinaire. Dans une phase smectique, les molécules sont organisées en couches : il existe donc, au-delà de l'ordre d'orientation, une forme d'ordre sur la position. Bien entendu, à l'intérieur de cette classification grossière plusieurs sous-cas sont possibles. Il existe aussi des situations intermédiaires parmi les nématiques et les sméctiques : par exemple, nous pouvons évoquer la phase *nématique hélicoïdale* (ou phase cholestérique), dans laquelle les molécules s'organisent de façon périodique, en hélice.

Dans tout ce travail, nous ne nous intéressons qu'aux phases nématiques (non cholestériques). De plus, nous supposerons que le matériau est composé de molécules allongées, possédant un axe de symétrie rotationnelle individué par un vecteur unitaire $\mathbf{n}$, et que la direction orientée $\mathbf{n}$ est équivalente à la direction $-\mathbf{n}$. Cette hypothèse est justifiée du point de vue expérimental parce que, même si les molécules sont associées à un dipôle électrique, il y a autant de molécules dans un sens que dans l'autre [38, 79]. Sous ces conditions, le groupe de symétrie des molécules est engendré par les rotations autour de l'axe directeur $\mathbf{n}$ et par la réflexion qui échange $\mathbf{n}$ et $-\mathbf{n}$. Nous parlons alors de nématiques *uniaxes*, par opposition aux nématiques biaxes pour lesquels les molécules ont le même groupe de symétrie qu'un rectangle. (Des preuves expérimentales de l'existence de nématiques biaxes ont été données d'abord pour des matériaux lyotropes [74], ensuite pour des thermotropes [94, 114]).

1.2 Les défauts : description homotopique

L'orientation des molécules dans les nématiques peut être observée au microscope, en plaçant un film mince de cristaux liquides entre deux surfaces en verre. En éclairant avec une lumière polarisée, on voit apparaître alors des textures colorées, que l'on appelle *schlieren textures*. Dans certains endroits, les molécules sont alignées perpendiculairement aux directions des polariseurs, donc ces endroits apparaissent noirs. En plusieurs points, l'orientation des molécules change de façon abrupte : il s'agit des *défauts* dans l'organisation des molécules. Puisque ces défauts portent sur l'orientation des molécules, ils sont aussi appelés *disinclinaisons* (disclinations, en anglais). Il est possible d'associer à chaque défaut un rang S, dit aussi charge topologique, de sorte que, en se déplaçant le long d'un circuit fermé orienté autour du défaut, le vecteur directeur du nématique tourne d'un angle $2\pi S$. Le nombre S est un demi-entier relatif ($S \in \{0, \pm 1/2, \pm 1, \pm 3/2, \ldots\}$).

Lorsque nous considérons un cristal liquide dans un domaine $\Omega \subset \mathbb{R}^3$, les défauts peuvent concerner des lignes aussi bien que des points. En fait, le mot même « nématique » fait référence aux défauts de ligne (Friedel, [49]) :

« *J'appellerai nématiques ($\nu\acute{\eta}\mu\alpha$, fil) les formes, phases, etc. du second type (Flüssige Kr.,*

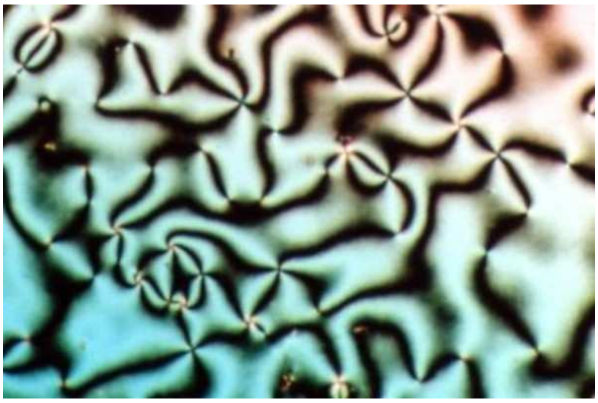
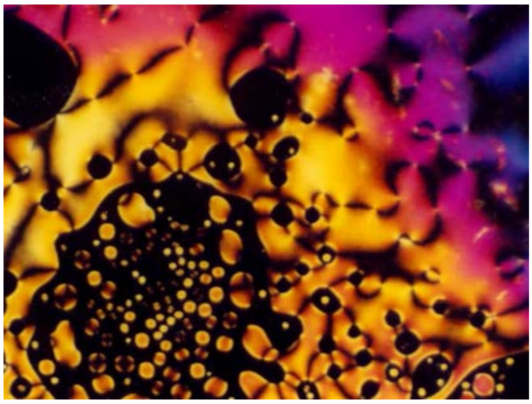
 

FIGURE 2 – Deux exemples de schlieren texture. Images réalisées par Minutemen (travail personnel), [GFDL, CC-BY-SA-3.0 ou CC BY-SA 2.5], via Wikimedia Commons.

> *Tropfbar flüssige Kr. de Lehmann : liquides à fils) à cause des discontinuités linéaires, contournées comme des fils, qui sont leurs caractères saillants.* »

Dans ce cas, décrire les défauts seulement à l'aide du rang S n'est plus satisfaisant. Il convient alors d'adopter une approche plus générale, qui fait appel aux groupes d'homotopie. Cette approche, introduite en 1976 par Toulouse et Kléman [139], Volovik et Mineev [142] et Rogula [120] et détaillée dans l'article de Mermin [99], repose sur une idée simple. Supposons que l'ensemble des configurations locales possibles pour le matériau soit une variété $\mathscr{N}$. Le milieu pourra alors être représenté par une fonction $u\colon \Omega \to \mathscr{N}$. Soient u, $u'\colon \Omega \to \mathscr{N}$ deux configurations, supposées continues sauf sur un ensemble $D \subset \mathbb{R}^3$ (le défaut). Supposons aussi que D est un ensemble régulier, disons une variété lisse. Les configurations u, u' seront considérés topologiquement équivalentes en D si et seulement si, pour tout couple de voisinages $D \subset\subset U \subset\subset V$, il existe une troisième configuration $v\colon \Omega \to \mathscr{N}$, continue sur $\Omega \setminus D$, telle que $v = u'$ sur U et $v = u$ sur $\Omega \setminus V$. En d'autres termes, u est équivalente à u' s'il est possible de remplacer la structure de u par celle de u' sur un voisinage du défaut, sans en modifier le comportement loin du défaut. La notion d'équivalence topologique entre deux configurations singulières revient alors à la notion d'homotopie entre applications continues. Plus précisément, une classe de configurations topologiquement équivalentes en D est caractérisée par la classe d'homotopie de l'application $u_{|C}\colon C \to \mathscr{N}$, où C est le bord de n'importe quel voisinage tubulaire de D. Si D est un point dans $\mathbb{R}^3$, alors C est une sphère autour de D. Si D est une ligne, alors C est (à difféomorphisme près) un cylindre $\mathbb{S}^1 \times \mathbb{R}$ et, puisque le cylindre rétracte par déformation sur la circonférence $\mathbb{S}^1$, nous pouvons nous ramener à l'étude de classes d'homotopie d'applications $\mathbb{S}^1 \to \mathscr{N}$.

Pour les nématiques uniaxes, les configurations possibles sont les droites non orientées passant par l'origine dans l'espace $\mathbb{R}^3$, correspondant aux directions qu'une molécule peut prendre. L'ensemble des droites, équipé d'une structure lisse convenable, constitue le plan projectif réel $\mathscr{N} = \mathbb{RP}^2$. En identifiant une ligne droite à l'opérateur de projection correspondant, nous pouvons assimiler $\mathbb{RP}^2$ à un ensemble de matrices :

$$\mathbb{RP}^2 := \left\{ \mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\colon \mathbf{n} \in \mathbb{S}^2 \right\} \subset \mathrm{M}_3(\mathbb{R}).$$

Nous avons introduit dans la définition un terme de renormalisation $-\,\mathrm{Id}/3$, comme il est d'usage dans la littérature sur les cristaux liquides. Avec cette convention, tout élément de $\mathbb{RP}^2$ est une matrice symétrique et à trace nulle, qui représente la déviation du milieu de l'état isotrope $\mathrm{Id}/3$. L'ensemble $\mathbb{RP}^2$ est une sous-variété lisse de l'espace $\mathrm{M}_3(\mathbb{R})$, de dimension 2. L'application $\psi\colon \mathbb{S}^2 \to \mathbb{RP}^2$ définie par

$$\psi(\mathbf{n}) := \mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \qquad \text{pour tout } \mathbf{n} \in \mathbb{S}^2$$

est lisse et surjective ; elle satisfait $\psi(\mathbf{n}) = \psi(-\mathbf{n})$. Cette application est le *revêtement universel* du plan

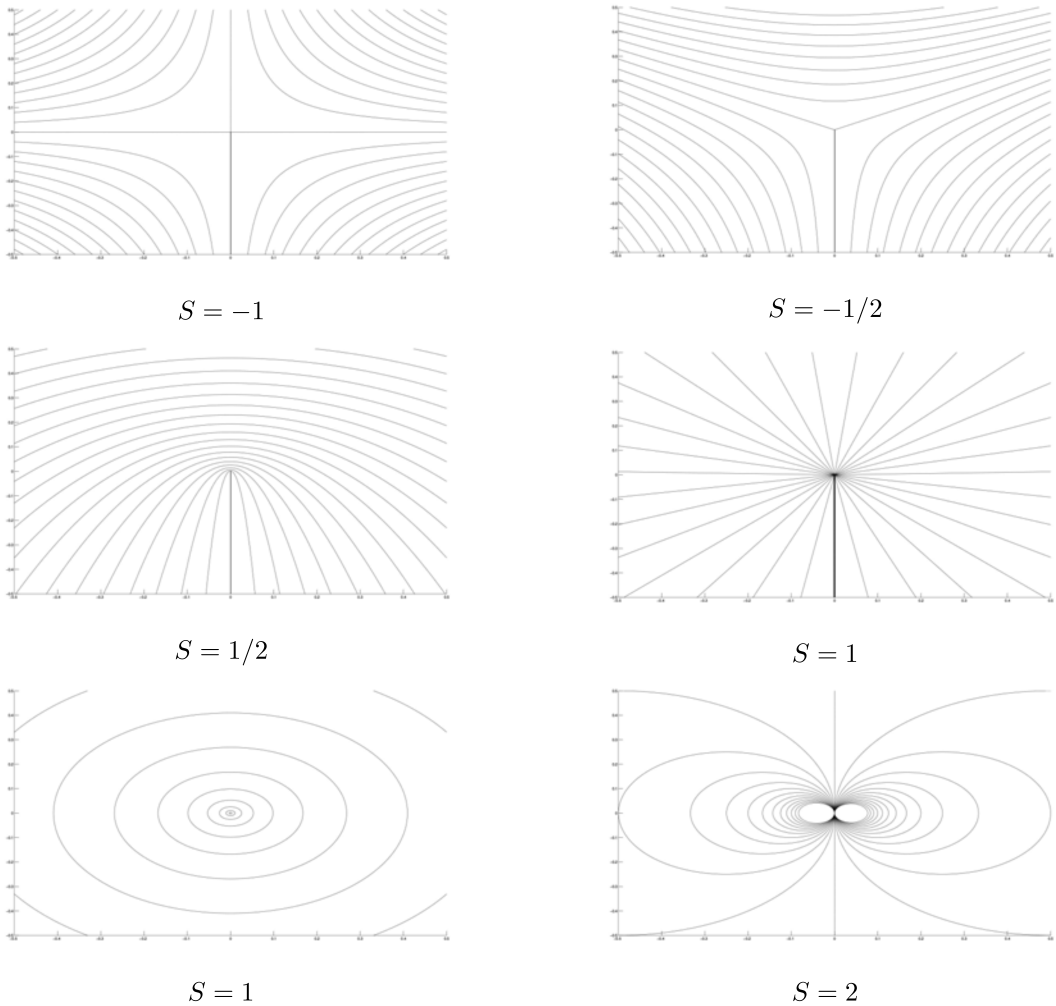


FIGURE 3 – Disinclinaisons dans une distribution planaire de nématiques.

projectif ; elle joue un rôle très important, car elle ramène l'étude des propriétés homotopiques du plan projectif à celles de la sphère $\mathbb{S}^2$.

Nous avons vu comment, dans une distribution des nématiques en dimension 3, les défauts de ligne et de point sont respectivement associés à des classes d'homotopie d'applications $\mathbb{S}^1 \to \mathscr{N}$ ou $\mathbb{S}^2 \to \mathscr{N}$. Ces classes correspondent *essentiellement* aux éléments des groupes d'homotopie $\pi_1(\mathscr{N})$ et $\pi_2(\mathscr{N})$. Le premier groupe d'homotopie est composé de deux éléments seulement :

$$\pi_1(\mathscr{N}) \simeq \mathbb{Z}/2\mathbb{Z}.$$

Notamment, une application $\gamma \in C^0(\mathbb{S}^1, \mathscr{N})$ est triviale (c'est-à-dire, homotope à une constante) si et seulement si elle peut être relevée, c'est-à-dire, s'il existe une application continue $\tilde{\gamma} \in C^0(\mathbb{S}^1, \mathbb{S}^2)$ telle que $\psi \circ \tilde{\gamma} = \gamma$. Cela revient à dire que le diagramme

$$\begin{tikzcd} & \mathbb{S}^2 \arrow[d, "\psi"] \\ \mathbb{S}^1 \arrow[ur, "\tilde{\gamma}"] \arrow[r, "\gamma"] & \mathscr{N} \end{tikzcd}$$

est commutatif. Pour tout point x, le vecteur $\tilde{\gamma}(x)$ définit une orientation pour la ligne associée à $\gamma(x)$; par conséquent, les applications qui admettent un relèvement sont aussi dites *orientables*. Donc, les seuls défauts de ligne topologiquement stables (c'est-à-dire, qui ne non pas topologiquement équivalents à des configurations non singulières) sont associés à la non-orientabilité du vecteur directeur du nématique.

Concernant le deuxième groupe d'homotopie, il s'avère que toute application continue $\gamma \in C^0(\mathbb{S}^2, \mathscr{N})$ admet un relèvement $\tilde{\gamma} \in C^0(\mathbb{S}^2, \mathbb{S}^2)$ (car $\mathbb{S}^2$ est simplement connexe ; voir, par exemple, [64, proposition 1.33 p. 61]). L'application qui associe à la classe d'homotopie de γ celle de son relèvement $\tilde{\gamma}$ définit un isomorphisme de groupes entre $\pi_2(\mathscr{N})$ et $\pi_2(\mathbb{S}^2)$ (voir [64, proposition 4.1 p. 342]) ; par conséquent,

$$\pi_2(\mathscr{N}) \simeq \mathbb{Z}.$$

Les défauts ponctuels dans un milieu nématique tridimensionnel se classifient donc par leur degré topologique.

La théorie homotopique permet aussi de décrire les défauts ponctuels dans une distribution planaire de nématiques. Si les molécules sont distribuées sur un plan $\Pi \subset \mathbb{R}^3$ passant par l'origine et si elles ne peuvent prendre que des directions contenues dans Π (comme dans le cas des « schlieren textures »), alors l'espace des configurations sera plutôt la droite projective réelle :

$$\mathscr{N} = \mathbb{RP}^1 := \left\{ \mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \colon \mathbf{n} \in \mathbb{S}^2 \cap \Pi \right\}.$$

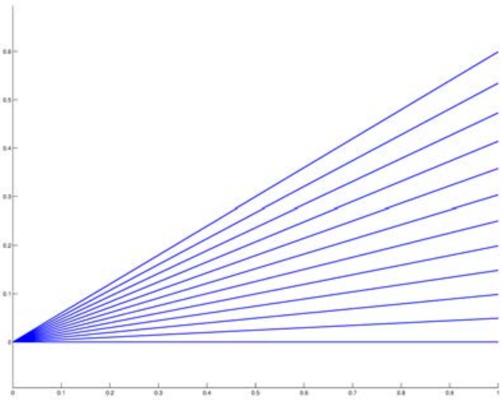
Il s'agit d'une variété lisse de dimension 1, difféomorphe à $\mathbb{S}^1$. Les défauts ponctuels sont caractérisés par les classes d'homotopie $C \to \mathbb{RP}^1$, où $C \subset \Pi$ est un cercle qui entoure le défaut. L'ensemble de telles classes constitue le groupe fondamental

$$\pi_1(\mathbb{RP}^1) \simeq \frac{1}{2}\mathbb{Z}$$

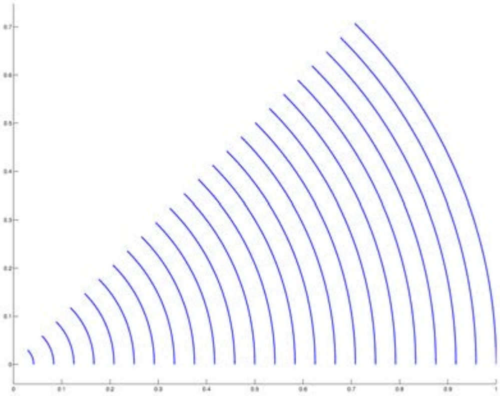
et chaque classe est identifiée par son rang ou charge topologique $S \in \frac{1}{2}\mathbb{Z}$, que nous avons défini précédemment. Par contre, si les molécules ne sont pas contraintes à rester sur le plan mais peuvent prendre toutes les directions dans $\mathbb{R}^3$, alors l'espace de configurations sera le plan projectif $\mathscr{N} = \mathbb{RP}^2$, comme dans le cas tridimensionnel. Dans ce cas, les défauts ponctuels seront représentés par les éléments du groupe fondamental $\pi_1(\mathbb{RP}^2)$.

Remarque 1. Par souci de précision, il convient de noter que l'identification entre les classes d'homotopie $\mathbb{S}^k \to \mathscr{N}$ (pour $k \in \mathbb{N}^*$) dont nous parlons ici et les éléments du groupe d'homotopie $\pi_k(\mathscr{N})$, pour une variété quelconque $\mathscr{N}$, n'est vraie qu'en première approximation. En effet, nous faisons référence ici à la notion d'homotopie *libre*, c'est-à-dire nous n'imposons aucune condition sur les points de base des applications. Au contraire, de telles conditions sont imposées dans la définition de $\pi_k(\mathscr{N})$. Néanmoins, les classes d'homotopie libre sont en bijection canonique avec les orbites de l'action de $\pi_1(\mathscr{N})$ sur $\pi_k(\mathscr{N})$ (voir, par exemple, [99, section VII.D p. 630]). Lorsque $k = 1$, le groupe fondamental agit sur lui-même par conjugaison. Les classes d'homotopie libre $\mathbb{S}^1 \to \mathscr{N}$ s'identifient alors aux classes de conjugaison dans $\pi_1(\mathscr{N})$; si $\pi_1(\mathscr{N})$ est abélien (comme il en est pour $\mathscr{N} \simeq \mathbb{RP}^2$), elles correspondent aux éléments du $\pi_1(\mathscr{N})$. Nous reviendrons sur ce fait dans le chapitre 1. Lorsque $k = 2$ et $\mathscr{N} \simeq \mathbb{RP}^2$, le groupe fondamental agit sur $\pi_2(\mathscr{N}) \simeq \mathbb{Z}$ comme le groupe d'automorphismes $\{\mathrm{Id}_{\mathbb{Z}}, -\mathrm{Id}_{\mathbb{Z}}\}$, donc les classes d'homotopie libre $\mathbb{S}^2 \to \mathscr{N}$ sont en bijection avec les nombres entiers modulo le signe.

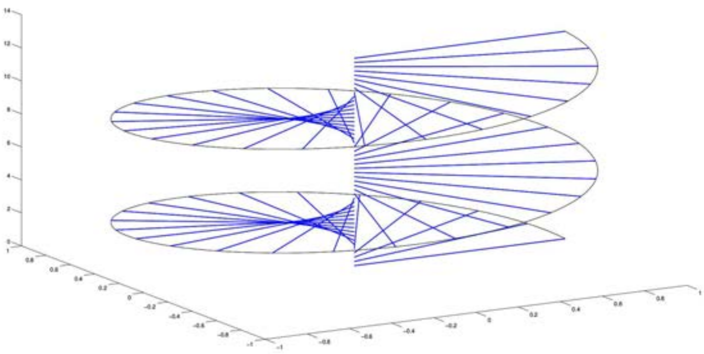
La classification homotopique des défauts donne des informations précieuses sur la nature des singularités que nous rencontrerons en étudiant les modèles variationnels pour les cristaux liquides. Ainsi, par exemple, la nature des données au bord peut forcer l'apparition d'un certain type de singularités. De plus, les configurations à caractère homotopiquement non triviale possèdent des énergies élastiques très élevées ; cela témoigne du lien entre description topologique et problèmes variationnels. Cependant, la présence de singularités dans les solutions n'est pas déterminée uniquement par la topologie. En effet, un défaut topologiquement instable — c'est-à-dire, qui est topologiquement équivalent à une configuration non singulière — peut être une configuration stable, ou même minimisante, du point de vue de l'énergie. Ce phénomène a été remarqué dans des contextes différents (par exemple, dans [62] ou [102] ; nous en reparlerons).



a) Splay ($\operatorname{div}\mathbf{n} \neq 0$)



b) Bend ($\mathbf{n} \times \operatorname{rot}\mathbf{n} \neq 0$)



c) Twist ($\mathbf{n} \cdot \operatorname{rot}\mathbf{n} \neq 0$)

FIGURE 4 – Déformations élastiques de divergence (a), de flexion (b) et de torsion (c).

2 Les cristaux liquides comme milieux continus : modèles variationnels

Dans cette section, nous présentons rapidement les principaux modèles variationnels pour les cristaux liquides qui relèvent de la mécanique des milieux continus. Il existe en effet des théories basées sur des approches différentes : par exemple, la théorie de Maier-Saupe, qui relève la mécanique statistique). Nous nous intéressons en particulier aux modèles d'Oseen-Frank et d'Ericksen, avant d'introduire le modèle de Landau-de Gennes qui sera l'objet principal de cette thèse.

2.1 Le modèle d'Oseen-Frank

Dans ce modèle, le milieu est décrit par un champ de vecteurs unitaires $\mathbf{n} = \mathbf{n}(x) \in \mathbb{S}^2$, qui représente le vecteur directeur du nématique au point $x \in \Omega \subset \mathbb{R}^3$. L'énergie élastique s'écrit

$$F_{\mathrm{OF}}(\mathbf{n}) := \frac{1}{2}\int_\Omega \sigma_{\mathrm{OF}}(\mathbf{n},\, \nabla\mathbf{n}), \tag{1}$$

où la densité d'énergie est donnée par

$$\sigma_{\mathrm{OF}}(\mathbf{n},\, \nabla\mathbf{n}) := \kappa_1 \left(\operatorname{div}\mathbf{n}\right)^2 + \kappa_2 \left(\mathbf{n}\cdot\operatorname{rot}\mathbf{n}\right)^2 + \kappa_3 \left|\mathbf{n}\times\operatorname{rot}\mathbf{n}\right|^2 + (\kappa_2+\kappa_4)\left\{\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2\right\}.$$

Les trois premiers termes prennent en compte des déformations élastiques de natures différentes : il s'agit respectivement des déformations de divergence (splay, en anglais), de flexion (bend) et de torsion (twist), illustrées dans la figure 4. Les constantes κ_i sont supposées satisfaire

$$2\kappa_1 \geq \kappa_2 + \kappa_4, \qquad \kappa_2 \geq |\kappa_4|\,, \qquad \kappa_3 \geq 0\ ;$$

ces inégalités forment des conditions nécessaires et suffisantes pour que l'on ait $\sigma_{\mathrm{OF}}(\mathbf{n},\, \nabla\mathbf{n}) \geq 0$ pour tout champ $\mathbf{n}$. Une dérivation phénoménologique de σ_{OF} est donnée en [38, 48, 140]. Dans *l'approximation à une constante* $\kappa_1 = \kappa_2 = \kappa_3 = \kappa$, la densité d'énergie prend la forme

$$\sigma_{\mathrm{OF}}(\mathbf{n},\, \nabla\mathbf{n}) = \kappa\,|\nabla\mathbf{n}|^2 + \kappa_4 \operatorname{div}\Big\{(\nabla\mathbf{n})\mathbf{n} - (\operatorname{div}\mathbf{n})\mathbf{n}\Big\}.$$

Après intégration sur Ω, le second terme se réduit à une intégrale de surface sur $\partial\Omega$, par application du théorème de Gauss-Green. Si ν est la normale sortante du bord de Ω, un simple calcul en coordonnées montre que $((\nabla\mathbf{n})\mathbf{n} - (\operatorname{div}\mathbf{n})\mathbf{n})\cdot\nu$ dépend seulement de $\mathbf{n}_{|\partial\Omega}$ et de ses dérivées tangentielles, donc il est complètement déterminé lorsqu'on assigne des conditions au bord de Dirichlet. Il suffit alors de considérer

$$F_{\mathrm{Dir}}(\mathbf{n}) := \frac{\kappa}{2}\int_\Omega |\nabla\mathbf{n}|^2\,, \tag{2}$$

qui est la fonctionnelle de Dirichlet. Les points critiques de cette fonctionnelle sont les applications harmoniques à valeurs dans la sphère unité $\mathbb{S}^2$. La littérature sur ce sujet est trop vaste pour être résumée ici ; nous ne rappelons que quelques résultats utiles pour la suite. Pour une présentation plus détaillée, le lecteur est renvoyé, par exemple, au rapport [70] et aux monographies [69, 107], consacrés au problème de la régularité partielle des applications harmoniques.

Les points critiques de (2) peuvent avoir un comportement très singulier : le travail de Rivière [117] montre qu'il existe des points critiques $\mathbf{n} \in H^1(B_1,\, \mathbb{S}^2)$ discontinus en tout point. La situation change radicalement si on s'intéresse aux minimiseurs. Schoen et Uhlenbeck [125, théorème II] ont démontré que tout minimiseur $\mathbf{n}$ de (2) est régulier sur $\Omega \setminus X$, où $X = \emptyset$ si le domaine est de dimension $N = 2$ et $X = X(\mathbf{n})$ est un ensemble fini si $N = 3$. Ce même résultat a été étendu aux points critiques de (2) satisfaisant une condition supplémentaire dite de stationnarité : il s'agit des travaux de Hélein [67, 68] pour le cas 2D, et d'Evans [45] et Bethuel [11] pour le 3D. De plus, en dimension 3 le comportement des minimiseurs au voisinage des points singuliers est connu. En effet, Brezis, Coron et Lieb [23, théorème 1.1] ont prouvé que, si $\mathbf{n}$ est un minimiseur de (2) et x_0 est un point singulier de $\mathbf{n}$, alors

$$\mathbf{n}(x) \simeq \pm R\frac{x - x_0}{|x - x_0|} \qquad \text{lorsque } |x - x_0| \ll 1, \tag{3}$$

où $R = R(x_0) \in \mathrm{SO}(3)$ est une rotation. En particulier, toutes les singularités sont de degré 1 ou -1. Une singularité de la forme (3) est appelée *hérisson*.

Des résultats intéressants ont aussi été prouvés pour les minimiseurs de (1). Lorsque $\Omega \subset \mathbb{R}^3$, Hardt, Kinderlehrer et Lin [60, théorèmes 1.5, 2.6 et 5.6] ont montré l'existence des minimiseurs (en imposant des conditions de Dirichlet au bord) et leur régularité partielle : pour tout minimiseur $\mathbf{n}$, il existe un ensemble fermé $X(\mathbf{n}) \subset \Omega$, de dimension de Hausdorff strictement inférieure à 1, tel que $\mathbf{n}$ est de classe C^∞ sur $\Omega \setminus X(\mathbf{n})$. Le comportement des minimiseurs au voisinage des singularités n'est pas aussi bien compris que dans le cas de l'approximation à une constante. On sait que l'application $x \mapsto |x|^{-1}x$ n'est *pas* minimisante si $8(\kappa_2 - \kappa_1) + \kappa_3 < 0$ (Hélein, [66]), et qu'elle est un point critique stable dans le cas contraire (Cohen et Taylor, [34]). Une étude plus complète de la stabilité du hérisson, qui prend également en compte la dépendance de R, est abordée dans [78] ainsi que dans les références qui y sont contenues.

2.2 Le modèle d'Ericksen

Dans le modèle d'Ericksen, le milieu est décrit par un couple de paramètres $(s,\, \mathbf{n}) \in [-1/2,\, 1] \times \mathbb{S}^2$, où $\mathbf{n}$ est le vecteur directeur moléculaire et s est le *paramètre d'ordre* scalaire, qui mesure le degré d'ordre moléculaire. La valeur $s = 1$ est associée à un état dans lequel toutes les molécules sont parallèles à $\mathbf{n}$; lorsque $s = 0$, la configuration est isotrope, c'est-à-dire complètement désordonnée, et il n'est pas possible de définir une direction privilégiée $\mathbf{n}$. Enfin, $s = -1/2$ représente une configuration dans laquelle toutes les molécules sont orthogonales à $\mathbf{n}$, mais orientées de façon désordonnée. En particulier, les défauts peuvent être caractérisés par les régions où $s = 0$. L'énergie est donnée par

$$F_{\mathrm{Er}}(s,\, \mathbf{n}) := \int_\Omega \left\{ \frac{1}{2}\sigma_{\mathrm{OF}}(\mathbf{n},\, \nabla\mathbf{n}) + \frac{1}{2}\sigma_{\mathrm{Er}}(\mathbf{n},\, \nabla s,\, \nabla\mathbf{n}) + \sigma_0(s) \right\}, \tag{4}$$

où

$$\sigma_{\mathrm{Er}}(\mathbf{n},\, \nabla s,\, \nabla\mathbf{n}) := \lambda_1 \left|\nabla s\right|^2 + \lambda_2 \left(\nabla s \cdot \mathbf{n}\right)^2 + \lambda_3 \left(\operatorname{div}\mathbf{n}\right)\left(\nabla s \cdot \mathbf{n}\right) + \lambda_4 \nabla s \cdot \left(\nabla\mathbf{n}\right)\mathbf{n}$$

et

$$\sigma_0(s) := \frac{a}{2}s^2 - \frac{b}{3}s^3 + \frac{c}{4}s^4 + d \tag{5}$$

(a, b, c, d étant fonctions strictement positives du matériau et de la température). L'expression pour la densité d'énergie élastique $\sigma_{\mathrm{OF}} + \sigma_{\mathrm{Er}}$ est dérivée du point de vue phénoménologique dans [44, 133, 140]. Le terme $\sigma_0(s)$ représente l'énergie potentielle, sous la forme proposée par de Gennes [38]. La fonction $s \mapsto \sigma_0(s)$ a deux minima locaux, en $s = 0$ (phase isotrope) et en $s = s_* > 0$ (phase orientée — voir la figure 5). Suivant la température, la fonction peut atteindre son maximum global en l'un ou l'autre point (ou les deux à la fois) ; par conséquent, l'une ou l'autre phase sera énergiquement plus favorable, ce qui induit la transition de phase isotrope-nématique. Les paramètres κ_i, λ_j satisfont des conditions convenables, qui assurent la positivité de la fonctionnelle.

Parmi les travaux portant sur la fonctionnelle (4), nous citons celui de Lin et Poon [88], qui établit l'existence de minimiseurs satisfaisant des conditions de Dirichlet au bord, pour un choix du potentiel σ_0 qualitativement différent de (5). La plupart des travaux se concentre sur le cas particulier où $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_E s^2$, $\kappa_4 = 0$, $\lambda_1 = \kappa_E \kappa$ et $\lambda_2 = \lambda_3 = \lambda_4 = 0$; dans ce cas-ci, la fonctionnelle prend la forme

$$F_{\mathrm{Es}}(s,\, \mathbf{n}) := \int_\Omega \left\{ \frac{\kappa_E}{2} \left(\kappa \left|\nabla s\right|^2 + s^2 \left|\nabla \mathbf{n}\right|^2 \right) + \sigma_0(s) \right\}. \tag{6}$$

Dans ce cadre simplifié, l'existence des minimiseurs pour le problème de Dirichlet est démontrée dans [5, 85, 86] pour tout σ_0 continu ; lorsque $\sigma_0 = 0$ et $0 < \kappa < 1$, on sait aussi que le minimiseur est unique (voir [86, théorème 4.1]). Avec le choix du potentiel (5), Lin [86, théorème 7.2] a démontré un résultat de régularité partielle : pour tout minimiseur $(s_0,\, \mathbf{n}_0)$, la fonction s_0 est localement lipschitzienne sur Ω alors que $\mathbf{n}$ est localement lipschitzienne sur $\Omega \setminus \mathscr{S}(s_0)$, où $\mathscr{S}(s_0) := s_0^{-1}(0)$. De plus, la dimension de Hausdorff de l'ensemble singulier $\mathscr{S}(s)$ est estimée par

$$\dim \mathscr{S}(s_0) \leq \begin{cases} 2 & \text{si } 0 < \kappa \leq 1 \\ 1 & \text{si } \kappa > 1. \end{cases} \tag{7}$$

Ensuite, Hardt et Lin [63, corollaire 3.4] ont prouvé que $\mathscr{S}(s_0)$ est un ensemble discret lorsque $\kappa > 1$. Dans le cas où $0 < \kappa \leq 1$, ce résultat de régularité partielle est compatible avec la présence de défauts de ligne ou de surface. En effet, de tels défauts apparaissent dans certains problèmes particuliers. Par exemple, Ambrosio et Virga [7] ont considéré une distribution de nématiques comprise entre deux plans parallèles Σ_+ et Σ_- en $\mathbb{R}^3$, avec des données au bord

$$\mathbf{n}_{|\Sigma_\pm} = (\cos\alpha)\mathbf{e}_1 \pm (\sin\alpha)\mathbf{e}_2, \qquad s_{|\Sigma_\pm} = s_1$$

(pour α, s_1 constantes positives et $(\mathbf{e}_1,\, \mathbf{e}_2)$ couple orthonormé de vecteurs parallèles à Σ_+, Σ_-). En supposant $\sigma_0 = 0$, lorsque κ est suffisamment petit par rapport à α le minimiseur s_0 s'annule sur un plan parallèle à Σ_+, Σ_-. Le même résultat a été démontré en prenant comme potentiel σ_0 une approximation de (5), voir [119]. Des défauts de ligne ont été observés pour une distribution de nématiques dans un cylindre $\Omega := B^2_R(0)\times(0,\, H)$. Mizel, Roccato et Virga [102] ont étudié les minimiseurs de (6) (pour $\sigma_0 = 0$) dans la classe des fonctions sous la forme

$$s = s(\rho), \qquad \mathbf{n} = (\cos\varphi(\rho))\,\mathbf{e}_\rho + (\sin\varphi(\rho))\,\mathbf{e}_z$$

(où $(\rho,\, \theta,\, z)$ dénotent les coordonnées cylindriques et $(\mathbf{e}_\rho,\, \mathbf{e}_\theta,\, \mathbf{e}_z)$ les vecteurs unitaires associés), avec conditions au bord $s(R) = s_1 > 0$, $\varphi(R) = 0$ pour s_1 constante. Dans cette classe, il existe un unique minimiseur $(s_0,\, \varphi_0)$. Lorsque $0 < \kappa \leq 1$, nous avons

$$s_0(\rho) = s_1\left(\frac{\rho}{R}\right)^{1/\sqrt{k}}, \qquad \varphi_0(\rho) = 0$$

donc la configuration minimisante présente un défaut de ligne sur l'axe du cylindre, de charge topologique $S = 1$. Par contre, si $\kappa > 1$ alors s_0 est partout strictement positif (donc il n'y a pas de défauts) et

$$\lim_{\rho\to 0^+} \varphi_0(\rho) = \frac{\pi}{2}\,;$$

cela indique que, bien que la donnée au bord soit perpendiculaire à l'axe du cylindre, pour $\rho = 0$ le vecteur directeur est parallèle à l'axe du cylindre. Ce phénomène est connu sous le nom d'échappement dans la troisième dimension.

Dans le modèle d'Ericksen, comme dans celui d'Oseen-Frank, la configuration du milieu est représentée à l'aide du vecteur directeur *orienté* $\mathbf{n} \in \mathbb{S}^2$. Cela ne prend pas en compte l'invariance par rapport à la symétrie $\mathbf{n} \mapsto -\mathbf{n}$, qui est suggérée par des considérations physiques, comme nous avons vu dans la sous-section 0.1.1. En plus, cela ne permet pas de décrire correctement les disinclinaisons de charge topologique non entière, qui sont associées à des défauts d'orientabilité. Pour remédier à ces inconvénients, Hardt et Lin [63, section 4] ont considéré une variante du modèle d'Ericksen, où l'inconnue $(s,\, \mathbf{n})$ prend ses valeurs en $[0,\, 1]\times\mathbb{RP}^2$. (La restriction $s \geq 0$ ne comporte pas une différence essentielle avec le modèle d'Ericksen : en effet, lorsque la donnée au bord satisfait $s \geq 0$, les minimiseurs de (6) satisfont aussi $s \geq 0$). Même dans ce cas, ils arrivent à démontrer l'estimation (7) sur la dimension de l'ensemble singulier.

Au-delà du problème d'orientabilité, les modèles d'Oseen-Frank et d'Ericksen reposent sur une hypothèse qui n'est pas complètement justifiée du point de vue physique : ils postulent qu'en chaque point de l'espace une direction d'orientation moléculaire privilégiée $\mathbf{n}$ est définie de façon unique. En effet, bien que les molécules — considérées individuellement — soient complètement décrites par leur axe de symétrie, quand on considère plusieurs molécules à la fois, des configurations plus compliquées peuvent apparaître. Ericksen même reconnaissait pour sa théorie un statut de « compromis »(voir [44, p. 100]) entre la simplicité mathématique et une description plus exhaustive de la réalité physique. Ce fut de Gennes qui, en reprenant des idées de Landau, proposa une théorie plus complète, en utilisant un formalisme matriciel. Cette théorie fut une des raisons qui lui valut le prix Nobel de physique, en 1991.

3 Le modèle de Landau-de Gennes

3.1 Les Q-tenseurs : interprétation statistique. Uniaxialité et biaxialité

Nous allons présenter ici les aspects principaux du modèle de Landau-de Gennes. Ce sujet est traité de façon plus approfondie dans la monographie de De Gennes et Prost [38], ainsi que dans le rapport de Mottram et Newton [108].

Considérons une distribution tridimensionnelle de nématiques uniaxes, au voisinage d'un point $x \in \mathbb{R}^3$. La distribution des molécules en fonction de l'orientation se décrit par une mesure de probabilité μ sur les boréliens $\mathscr{B}(\mathbb{S}^2)$, satisfaisant la contrainte de symétrie moléculaire

(8) $$\mu(B) = \mu(-B) \qquad \text{pour tout } B \in \mathscr{B}(\mathbb{S}^2).$$

Nous voulons condenser les informations contenues dans μ dans une quantité qu'on puisse traiter plus facilement. Une solution — inspirée par la mécanique des milieux continus — est de considérer les moments de la probabilité μ. Or le moment d'ordre zéro, la densité, ne porte aucune information sur la distribution en orientation de molécules, et celui d'ordre un s'annule à cause de (8). Donc, le premier moment significatif à considérer est celui d'ordre deux :

$$Q := \int_{\mathbb{S}^2} \left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right) \mathrm{d}\mu(\mathbf{p}). \tag{9}$$

En suivant la convention établie par de Gennes, nous avons introduit un terme de renormalisation, de sorte que le moment associé à la distribution isotrope $\mu \propto \mathscr{H}^2 \llcorner \mathbb{S}^2$ soit $Q = 0$. Le moment Q est une matrice 3×3 réelle, symétrique et à trace nulle. Une telle matrice est dite un *Q-tenseur*. Par la suite, nous noterons

$$\mathbf{S}_0 := \left\{ Q \in \mathrm{M}_3(\mathbb{R}) \colon Q = Q^{\mathsf{T}}, \ \mathrm{tr}\, Q = 0 \right\}$$

l'espace des Q-tenseurs : il s'agit d'un espace vectoriel réel, de dimension 5, sur lequel nous définissons un produit scalaire par $Q \cdot P := Q_{ij}P_{ij}$. Notons que toute matrice obtenue par la formule (9) satisfait une contrainte sur les valeurs propres $\lambda_1 \geq \lambda_2 \geq \lambda_3$:

$$-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3} \qquad \text{pour } i \in \{1,\, 2,\, 3\}. \tag{10}$$

Les Q-tenseurs se classifient suivant leurs valeurs propres. Nous dirons qu'un Q-tenseur est

(i) *isotrope*, si $Q = 0$;

(ii) *uniaxe*, si $Q \neq 0$ et deux valeurs propres coïncident ;

(iii) *biaxe*, si toutes les valeurs propres sont différentes.

Ces classes de tenseurs correspondent à des propriétés de symétrie différentes sur la mesure μ. En effet, pour tout Q-tenseur vérifiant (10) il existe une mesure de probabilité μ sur $\mathscr{B}(\mathbb{S}^2)$, qui satisfait (8), (9) et les conditions suivantes.

(i) Si Q est isotrope, alors μ est la distribution uniforme, c'est-à-dire

$$\mu = \mu_0 := \frac{1}{4\pi}\mathscr{H}^2 \llcorner \mathbb{S}^2.$$

(ii) Si Q est uniaxe, alors μ admet un axe de symétrie rotationnelle. En d'autres termes, il existe un vecteur unitaire $\mathbf{n}$ tel que, pour toute rotation $R \in \mathrm{SO}(3)$ satisfaisant $R\mathbf{n} = \mathbf{n}$,

$$\mu(R(B)) = \mu(B) \qquad \text{pour tout } B \in \mathscr{B}(\mathbb{S}^2).$$

(iii) Si Q est biaxe, alors il existe un repère orthogonale $(\mathbf{n},\, \mathbf{m},\, \mathbf{p})$ tel que, si $S \in \mathrm{SO}(3)$ est une symétrie axiale d'axe $\mathbf{n}$, $\mathbf{m}$ ou $\mathbf{p}$, alors

$$\mu(S(B)) = \mu(B) \qquad \text{pour tout } B \in \mathscr{B}(\mathbb{S}^2).$$

Une preuve de ce fait sera donnée dans le chapitre 1 (lemme 1.3.2). Dans toute cette thèse, on parlera d'uniaxialité ou biaxialité au sens indiqué ci-dessus ; à savoir, le caractère uniaxe et biaxe concernera toujours les *configurations* des molécules et non les molécules elles-mêmes, qui seront toujours supposées uniaxes.

Étant donnée une matrice $Q \in \mathbf{S}_0 \setminus \{0\}$, il est possible d'écrire Q sous la forme suivante :

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right) + sr\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right), \tag{11}$$

où $s > 0$, $0 \leq r \leq 1$ et $(\mathbf{n}, \mathbf{m})$ est un couple de vecteurs orthonormés dans $\mathbb{R}^3$. Les nombres s et r sont déterminés de manière univoque. Cette formule de représentation, qui est une variante d'une formule classique (voir, par exemple, [98, proposition 1]), sera prouvée dans le chapitre 1 (lemma 1.3.1). Remarquons aussi que la matrice Q est uniaxe si et seulement si $r = 0$ ou $r = 1$; dans ce dernier cas, en utilisant l'identité $\mathrm{Id} = \mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2} + \mathbf{p}^{\otimes 2}$ où $\mathbf{p} := \mathbf{n} \times \mathbf{m}$, nous pouvons voir que

$$Q = -s\left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right).$$

Il existe deux classes de matrices uniaxes : les matrices uniaxes « allongés »(*prolate* uniaxial, en anglais), pour lesquelles la valeur propre dominante est simple (c'est-à-dire $\lambda_1 > \lambda_2 = \lambda_3$), et les matrices « aplaties »(*oblate* uniaxial) pour lesquelles la valeur propre dominante est double, $\lambda_1 = \lambda_2 > \lambda_3$. La nomenclature fait référence à l'ellipsoïde de révolution associé à la matrice. Comme nous le verrons dans le chapitre 1, ces deux classes correspondent au cas $r = 0$ et $r = 1$, respectivement.

3.2 La fonctionnelle d'énergie

L'énergie associée à la configuration Q dans un domaine $\Omega \subset \mathbb{R}^N$ (pour $N \in \{2, 3\}$) s'écrit

$$F_{\mathrm{LdG}}(Q) := \int_\Omega \left\{\sigma_{\mathrm{LdG}}(Q, \nabla Q) + f(Q)\right\},$$

où σ_{LdG} est la densité d'énergie élastique, qui pénalise les déviations de l'homogénéité spatiale, et f est un potentiel qui induit la transition de phase isotrope-nématique. La densité d'énergie élastique doit être invariante par changement de repère des coordonnées et par réflexion, puisque les milieux nématiques sont achirales. Ces deux contraintes peuvent s'exprimer en disant que, pour tout $R \in \mathrm{O}(3)$, la densité d'énergie élastique satisfait

$$\sigma_{\mathrm{LdG}}(Q^*, D^*) = \sigma_{\mathrm{LdG}}(Q, \nabla Q) \qquad \text{où } Q^*_{ij} := R_{ip}R_{jq}Q_{pq},\ D^*_{ijk} := R_{im}R_{jp}R_{kq}Q_{mp,q} \tag{12}$$

(ici et par la suite, nous utilisons la notation $Q_{mp,q} := \partial_q Q_{mp}$). Un exemple de densité quadratique en ∇Q qui satisfait (12) a été proposé par de Gennes [37] :

$$\sigma_{\mathrm{LdG}}(Q, \nabla Q) = L_1 Q_{ij,j}Q_{ik,k} + L_2 Q_{ij,k}Q_{ik,j} + L_3 Q_{ij,k}Q_{ij,k} + L_4 Q_{kl}Q_{ij,k}Q_{ij,l}. \tag{13}$$

Les constantes élastiques L_i sont liées aux constantes κ_i de la théorie d'Oseen-Frank : en effet, un calcul formel à partir de l'ansatz $Q = s(\mathbf{n}^{\otimes 2} - \mathrm{Id}/3)$ montre que $\sigma_{\mathrm{LdG}}(Q, \nabla Q) = \sigma_{\mathrm{OF}}(\mathbf{n}, \nabla \mathbf{n})$, à condition que

$$\frac{\kappa_1}{s^2} = 2L_1 + L_2 + L_3 - \frac{2}{3}L_4 s, \quad \frac{\kappa_2}{s^2} = 2L_1 - \frac{2}{3}L_4 s, \quad \frac{\kappa_3}{s^2} = 2L_1 + L_2 + L_3 + \frac{4}{3}L_4 s, \quad \frac{\kappa_4}{s^2} = L_3.$$

Quant au potentiel f, il faut bien qu'il soit aussi invariant par rotations et réflexions :

$$f(Q) = f(RQR^{\mathsf{T}}) \qquad \text{pour tout } R \in \mathrm{SO}(3).$$

Par conséquent, f doit être une fonction des invariants scalaires de Q, qui à leur tour s'expriment en fonction de $\operatorname{tr} Q^2$, $\operatorname{tr} Q^3$ en utilisant le fait que $\operatorname{tr} Q = 0$. Inspiré par une remarque de Landau, de Gennes [37, 38] a proposé pour f la forme suivante :

$$f(Q) := k_0 + \frac{\alpha}{2}(T - T_*)\operatorname{tr} Q^2 - \frac{\beta}{3}\operatorname{tr} Q^3 + \frac{\gamma}{4}\left(\operatorname{tr} Q^2\right)^2, \tag{14}$$

où T est la température du milieu (qu'on suppose constante et homogène), T_* est une température caractéristique du matériau et α, β, γ sont des paramètres strictement positifs dépendant du matériau. La constante k_0 ne joue aucun rôle par la suite ; pour l'instant, nous supposons que $k_0 = 0$. En utilisant

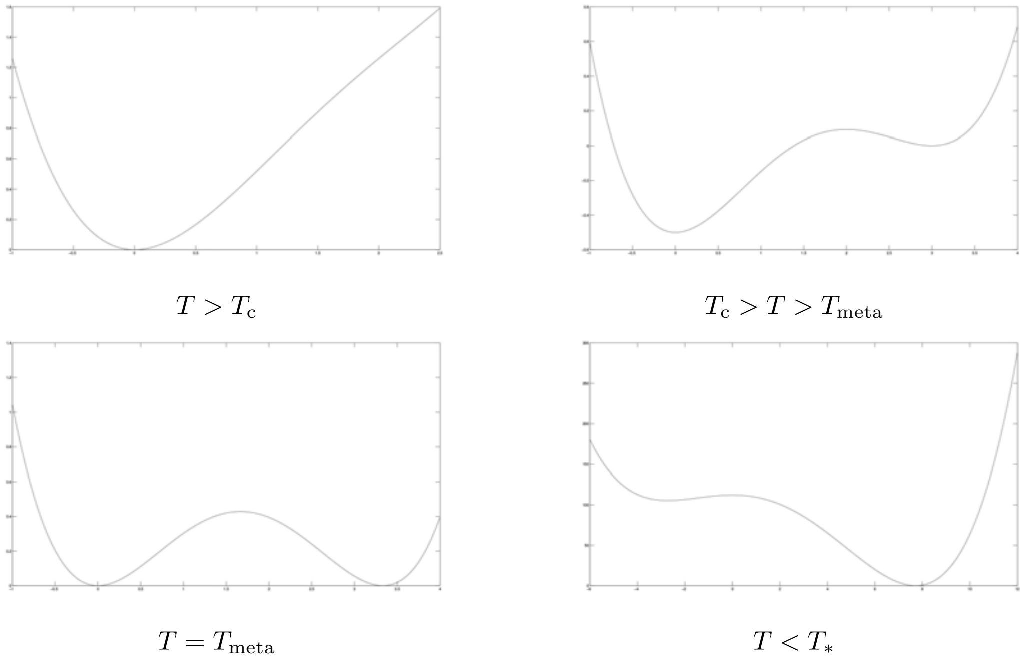


FIGURE 5 – La fonction $s \mapsto g_T(s)$, pour quelques valeurs de la température T.

encore l'ansatz uniaxe $Q = s(\mathbf{n}^{\otimes 2} - \mathrm{Id}/3)$, nous pouvons écrire f en fonction du paramètre d'ordre scalaire s :

$$f(Q) = g_T(s) := \frac{\alpha}{3}(T - T_*)s^2 - \frac{2\beta}{27}s^3 + \frac{\gamma}{9}s^4.$$

Le comportement des phases stables, qui correspondent aux minima locaux de $s \mapsto g(s)$, varie avec la température, comme illustré dans la figure 5.

◇ Lorsque $T > T_{\mathrm{c}} := T_* + \dfrac{\beta^2}{24\alpha\gamma}$, le seul point critique de g_T est $s = 0$ (phase isotrope).

◇ Lorsque $T_{\mathrm{c}} \geq T > T_*$, un deuxième point critique apparaît en

$$s = s_*(T) := \frac{\beta + \sqrt{\beta^2 + 24\alpha\gamma(T_* - T)}}{4\gamma}, \tag{15}$$

correspondant à une phase nématique ordonnée. Ce point critique est instable pour $T = T_{\mathrm{c}}$ (car g_T est croissante dans un voisinage de $s_*(T_{\mathrm{c}})$), mais il devient stable dès que $T < T_{\mathrm{c}}$. L'origine reste un point critique stable. Dans ce régime de température, les phases nématique et isotrope coexistent dans le système.

◇ Lorsque $T \leq T_*$, la phase isotrope $s = 0$ perd sa stabilité, en faveur de la phase nématique $s = s_*(T)$. La transition de phase est donc complétée ; le mésogène est dans la phase nématique.

La fonction $T \mapsto g_T(s(T))$ est continue et strictement décroissante. Il existe donc une valeur T_{meta} telle que $g_{T_{\mathrm{meta}}}(s_*(T_{\mathrm{meta}})) = g_{T_{\mathrm{meta}}}(0) = 0$. Pour cette valeur de la température, les phases isotrope et nématique sont également favorables du point de vue de l'énergie : on parle de phases *métastables*. Le potentiel quartique, donné par la formule (14), est le plus simple potentiel polynomial en Q qui engendre une transition de phase « à régime mixte », du type que nous avons décrit ici.

Ball et Majumdar [9, proposition 4] ont remarqué que, en couplant la densité d'énergie élastique (13) avec le potentiel (14), il en résulte une fonctionnelle non bornée inférieurement dès que $L_4 \neq 0$. En effet, nous avons

$$\begin{aligned}\psi_{\mathrm{LdG}}(Q,\,\nabla Q) &= L_1 Q_{ij,j}Q_{ik,k} + L_2 Q_{ij,k}Q_{ik,j} + \left(L_3 - \frac{L_4}{3}\right) Q_{ij,k}Q_{ij,k} + L_4\left(Q_{kl} + \frac{\delta_{kl}}{3}\right) Q_{ij,k}Q_{ij,l} \\ &\leq C\,|\nabla Q|^2 + L_4\left(Q + \frac{\mathrm{Id}}{3}\right)\nabla Q_{ij}\cdot\nabla Q_{ij}\end{aligned}$$

et le dernier terme tend vers $-\infty$ lorsque les valeurs propres de Q tendent vers $-\infty$. Dans le même article, Ball et Majumdar ont proposé un potentiel singulier, tel que $f(Q) = +\infty$ si Q ne satisfait pas la contrainte sur les valeurs propres (10). Avec leur choix de f, la fonctionnelle F_{LdG} reste bornée inférieurement même pour $L_4 \neq 0$. D'autre part, le traitement mathématique du problème qui en résulte est compliqué, à cause de la singularité du potentiel de Ball et Majumdar (pour lequel on ne dispose pas d'une formule explicite). De plus, le terme cubique présent dans σ_{LdG} est délicat à traiter.

Dans toute cette thèse, nous nous intéresserons au cas où $L_1 = L_2 = L_4 = 0$, pour lequel σ_{LdG} se réduit à $L_3|\nabla Q|^2$. Malgré sa simplicité, ce problème possède déjà une structure riche. Nous supposons aussi que $T < T_*$ (la transition de phase est complétée, la phase nématique est la seule phase minimisante). En posant $\varepsilon := (2L_3)^{1/2}$, nous pouvons nous ramener à l'étude de la fonctionnelle

$$E_\varepsilon(Q) := \int_\Omega \left\{\frac{1}{2}\,|\nabla Q|^2 + \frac{1}{\varepsilon^2} f(Q)\right\} \tag{LG$_\varepsilon$}$$

où

$$f(Q) = k_0 - \frac{a}{2}\,\mathrm{tr}\,Q^2 - \frac{b}{3}\,\mathrm{tr}\,Q^3 + \frac{c}{4}\left(\mathrm{tr}\,Q^2\right)^2 \tag{16}$$

(nous avons posé $a := \alpha(T_* - T) > 0$, $b := \beta > 0$, $c := \gamma > 0$). Nous choisissons $k_0 = k_0(a,\,b,\,c)$ de sorte que $\inf f = 0$. La constante élastique ε^2 est généralement assez petite (nous avons $\varepsilon^2 \simeq 10^{-11}$ Jm^{-1} comme ordre de grandeur dans plusieurs cas concrets) ; par la suite, nous supposerons que

$$0 < \varepsilon < 1.$$

On remarquera que nous n'avons pas du tout pris en compte les effets des champs électriques et magnétiques ici. Afin que les minimiseurs ne soient pas triviaux, il convient alors de coupler (LG$_\varepsilon$) avec des conditions au bord. Nous choisissons ici des conditions de Dirichlet non homogènes : étant donné $g \in H^{1/2}(\partial\Omega,\,\mathbf{S}_0)$, nous cherchons les minimiseurs de (LG$_\varepsilon$) dans la classe

$$H^1_g(\Omega,\,\mathbf{S}_0) := \left\{Q \in H^1(\Omega,\,\mathbf{S}_0)\colon Q_{|\partial\Omega} = g_{|\partial\Omega} \text{ au sens des traces}\right\}.$$

Bien qu'éloigné de la formulation générale du modèle physique, le problème de Dirichlet pour la fonctionnelle (LG$_\varepsilon$) a été beaucoup traité dans la littérature mathématique des cristaux liquides (voir, par exemple, [41, 51, 71, 73, 83, 98]). Remarquons tout de suite que des minimiseurs existent par un argument classique de calcul de variations, et sont réguliers en tant que solutions de l'équation d'Euler-Lagrange associée à (LG$_\varepsilon$).

L'ensemble des minimiseurs de f, à savoir

$$\mathscr{N} := \{Q \in \mathbf{S}_0\colon f(Q) = \inf f\},$$

joue un rôle important dans le problème. Cet ensemble peut être caractérisé de la façon suivante :

$$\mathscr{N} = \left\{s_*\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) : \mathbf{n} \in \mathbb{S}^2\right\} \tag{17}$$

(voir [98, proposition 9]), où $s_* = s_*(T)$ a été défini en (15). Il s'agit donc d'une variété lisse, difféomorphe au plan projectif $\mathbb{RP}^2$, qu'on appellera *variété du vide.* Lorsque ε est très petit, les minimiseurs de (LG$_\varepsilon$)

sont forcés de prendre leurs valeurs aussi proches que possible de $\mathscr{N}$. Or, la topologie non triviale de $\mathscr{N}$ implique, dans certains cas, une obstruction à l'existence d'applications régulières $\Omega \to \mathscr{N}$ satisfaisant la condition au bord ; alors, lorsque $\varepsilon \to 0$, on peut s'attendre à que le minimiseurs convergent vers des applications $\Omega \to \mathscr{N}$ ayant des singularités. Les sources de cette obstruction sont les groupes d'homotopie $\pi_1(\mathscr{N}) \simeq \mathbb{Z}/2\mathbb{Z}$ et $\pi_2(\mathscr{N}) \simeq \mathbb{Z}$, respectivement associés à des singularités de codimension 2 et 3. La formulation variationnelle du problème permet donc de récupérer les informations issues de la théorie homotopique des défauts, présentée dans la sous-section 0.1.2.

Puisque la variété du vide est le plan projectif, la théorie de Landau-de Gennes prend en compte les défauts d'orientabilité, contrairement à la théorie d'Oseen-Frank et à celle d'Ericksen. Malgré cette différence, un lien fort entre la théorie de Landau-de Gennes et celle d'Oseen-Frank a été établi par Majumdar et Zarnescu. Dans leur papier [98], ils étudient le comportement asymptotique des minimiseurs de $(\mathrm{LG}_\varepsilon)$, sur des domaines tridimensionnels, lorsque $\varepsilon \to 0$. Ils prouvent que, si Ω, $\partial\Omega$ sont simplement connexes et la donnée au bord g (indépendante de ε) satisfait $g \in C^1(\partial\Omega, \mathscr{N})$, alors les minimiseurs Q_ε convergent dans $H^1(\Omega, \mathbf{S}_0)$ à une application de la forme

$$Q_0(x) = s_* \left(\mathbf{n}_0^{\otimes 2}(x) - \frac{1}{3}\,\mathrm{Id}\right),$$

où $\mathbf{n}_0 \in H^1(\Omega, \mathbb{S}^2)$ est un minimiseur de l'énergie de Dirichlet (2). De plus, la convergence est localement uniforme, loin des singularités de $\mathbf{n}_0$. Dans ces conditions, le résultat de régularité partielle de Schoen et Uhlenbeck [125] interdit les singularités de ligne, bien qu'il puisse y avoir des défauts ponctuels de type hérisson. En effet, les hypothèses sous lesquelles Majumdar et Zarnescu se placent sont suffisamment fortes pour garantir l'existence d'une application $P \in H^1(\Omega, \mathscr{N})$ satisfaisant les conditions au bord. Un argument de comparaison donne alors

$$E_\varepsilon(Q_\varepsilon) \leq C \tag{18}$$

pour une constante C indépendante de ε, ce qui entraîne la compacité dans H^1. Par contre, nous verrons par la suite que la formation de singularités de codimension 2 à la limite $\varepsilon \to 0$ est associée au régime d'énergie logarithmique :

$$E_\varepsilon(Q_\varepsilon) \leq C\left(|\log\varepsilon| + 1\right). \tag{19}$$

3.3 Comparaison avec le modèle de Ginzburg-Landau

En écrivant la fonctionnelle de Landau-de Gennes sous la forme $(\mathrm{LG}_\varepsilon)$, on voit très nettement l'analogie avec la fonctionnelle de Ginzburg-Landau, qui modélise l'énergie libre des supraconducteurs. Si l'on néglige les champs électriques et magnétiques, cette énergie prend la forme

$$E_\varepsilon^{\mathrm{GL}}(u) := \int_\Omega \left\{\frac{1}{2}\left|\nabla u\right|^2 + \frac{1}{4\varepsilon^2}\left(1 - |u|^2\right)^2\right\}, \tag{20}$$

pour une fonction $u\colon \Omega \to \mathbb{C}$. La variété du vide associée à ce modèle est le lieu d'annulation de $u \mapsto (1-|u|^2)^2$, c'est-à-dire le cercle unité $\mathbb{S}^1$. La seule obstruction topologique à la régularité provient du groupe fondamental $\pi_1(\mathbb{S}^1) \simeq \mathbb{Z}$.

Il existe une littérature riche consacrée au comportement asymptotique, lorsque $\varepsilon \to 0$, des points critiques de (20) satisfaisant une majoration logarithmique pour l'énergie, telle que (19). Sous des hypothèses adéquates, ces points critiques convergent à des applications $\Omega \to \mathbb{S}^1$ ayant des singularités topologiques de codimension 2. Pour des domaines étoilés en dimension $N = 2$, cela a été démontré par Bethuel, Brezis et Hélein [14] ; ensuite, ce résultat a été généralisé par Struwe [136] aux domaines bornés réguliers quelconques (une preuve simple a été donnée par del Pino et Felmer [40]). Dans le cas $N \geq 3$, l'analyse asymptotique a été conduite d'abord pour le minimiseurs (Lin et Rivière, [89]) et ensuite pour les points critiques non minimisants (Bethuel, Brezis et Orlandi, [15]). Une étape ultérieure dans la compréhension du problème a été l'étude de la Γ-convergence pour la fonctionnelle renormalisé

$$I_\varepsilon(u) := |\log\varepsilon|^{-1} E_\varepsilon^{\mathrm{GL}}(u).$$

Jerrard et Soner [76] et Alberti, Baldo, Orlandi [2] ont prouvé indépendamment que $I_\varepsilon \to I_0$ au sens de la Γ-convergence, lorsque $\varepsilon \to 0$. La fonctionnelle I_0, définie sur l'espace des courants intégraux de codimension 2, mesure la masse $(N-2)$-dimensionnelle des défauts, pondérée par une quantité qui prend en compte leur caractéristiques topologiques. La topologie par rapport à laquelle la Γ-convergence a lieu est induite par la convergence faible-$*$ des jacobiens. En effet, si $\{u_\varepsilon\}_{\varepsilon>0}$ est une famille telle que $\liminf_{\varepsilon\to 0} I_\varepsilon(u_\varepsilon) < +\infty$ alors, quitte à extraire une sous-suite $\{\varepsilon_n\}_{n\in\mathbb{N}}$, nous avons la convergence

$$\mathrm{J}u_{\varepsilon_n} := \star\left(\mathrm{d}u^1_{\varepsilon_n} \wedge \mathrm{d}u^2_{\varepsilon_n}\right) = \frac{1}{2} \star \mathrm{d}\left(u^1_{\varepsilon_n}\mathrm{d}u^2_{\varepsilon_n} - u^2_{\varepsilon_n}\mathrm{d}u^1_{\varepsilon_n}\right) \rightharpoonup^* \pi J_0 \qquad \text{dans } C^{0,\alpha}_c\left(\Omega,\, \Lambda^{N-2}\mathbb{R}^N\right)',$$

où $\star$ dénote l'opérateur de dualité de Hodge et J_0 est un $(N-2)$-courant intégral.

Une généralisation intéressante du modèle de Ginzburg-Landau a été proposée par Chiron dans son travail de thèse [33]. Il s'agit de considérer la même fonctionnelle (20), cette fois-ci pour des applications $u\colon \Omega \to X(\mathscr{M})$ où $\mathscr{M}$ est une variété (lisse et compacte) arbitraire, et $X(\mathscr{M})$ est le *cône construit sur* $\mathscr{M}$:

$$X(\mathscr{M}) := ((0,\, +\infty) \times \mathscr{M}) \cup \{0\}, \tag{21}$$

avec une métrique définie en conséquence. Le modèle de Ginzburg-Landau correspond au choix $\mathscr{M} = \mathbb{S}^1$; lorsque $\mathscr{M} = \mathbb{S}^2$, nous obtenons un modèle proche de celui d'Ericksen. En dimension 2, Chiron a prouvé la convergence des minimiseurs vers des applications ayant des singularités ponctuelles.

Bien que les fonctionnelles $(\mathrm{LG}_\varepsilon)$ et (20) soient semblables, il existe des différences remarquables entre les deux modèles. Parmi les plus frappantes, nous signalons que, dans le modèle de Ginzburg-Landau (et aussi dans sa version généralisée proposée par Chiron), la variété du vide $\mathbb{S}^1 \subset \mathbb{C}$ est de codimension 1, alors que dans le modèle de Landau-de Gennes elle est de codimension 3. Par conséquent, pour les minimiseurs de Ginzburg-Landau les défauts sont caractérisés par les régions où $|u| \simeq 0$; en revanche, pour les minimiseurs de Landau-de Gennes plusieurs comportements sont possibles, et le passage par la phase isotrope peut être évité par un « échappement dans les phases biaxes ».

4 Biaxialité dans le modèle de Landau-de Gennes

Nous avons vu que la variété du vide $\mathscr{N}$ est composée de matrices uniaxes (voir (17)). Loin des défauts, le résultat de convergence uniforme de Majumdar et Zarnescu [98, propositions 5 et 7] (ainsi que les résultats présentés dans la section 0.5) implique que les minimiseurs Q_ε sont très proches de la phase purement uniaxe, pour ε petit. En revanche, dans le noyau des défauts, les minimiseurs peuvent avoir un comportement isotrope ou biaxe. Nous nous intéressons ici à la question : *est-ce que la biaxialité est présente dans les configurations minimisantes, pour* $\varepsilon > 0$ *petit* ?

Le phénomène d'« échappement dans les phases biaxes », qui permet d'éviter la présence de phases isotropes dans le coeur des singularités, a été identifié par Lyuksyutov [93]. Son travail, suivi de celui de Penzenstadler et Trebin [112], suggère que la biaxialité est privilégiée lorsque le coefficient du terme cubique b dans le potentiel (16) est petit. Tel est le cas si la température est basse. Définissons la *température réduite*

$$t := \frac{ac}{b^2} \propto T_* - T > 0. \tag{22}$$

Si la température T est basse alors t prend une valeur élevée, donc le coefficient b est petit par rapport aux autres.

Dans la littérature, il existe déjà plusieurs résultats qui impliquent la biaxialité des minimiseurs lorsque $t \gg 1$. Gartland et Mkaddem [51] ont remarqué que, dans une boule $B_R \subset \mathbb{R}^3$, le hérisson uniaxe — défini comme l'unique point critique de $(\mathrm{LG}_\varepsilon)$ uniaxe et à symétrie radiale — devient instable pour $t \gg 1$. Dans [73, théorème 1.2], Ignat et al. ont démontré que le hérisson est également instable dans l'espace tout entier $\mathbb{R}^3$, lorsque $t \gg 1$ (mais stable si $t \ll 1$). Henao et Majumdar [71, théorème 1] ont prouvé que tout point critique uniaxe est instable si $t \gg 1$. En effet, Lamy [83, théorèmes 4.1 et 5.1] a montré plus tard que le hérisson uniaxe est le seul point critique uniaxe ; le résultat de Henao et Majumdar s'obtient alors en combinant le théorème de Lamy avec la remarque de Gartland et Mkaddem. Dans le même travail, Lamy a aussi prouvé que, en dimension 2, les seuls points critiques purement uniaxes ont la forme

$$Q(x) = s(x) \left(\mathbf{n}_0^{\otimes 2} - \frac{1}{3} \,\mathrm{Id} \right)$$

où $\mathbf{n}_0 \in \mathbb{S}^2$ est une constante. En particulier, il n'existe pas de points critiques uniaxes si les conditions au bord sont non triviales. Des simulations numériques (Schopohl et Sluckin, [128]) suggèrent que le noyau des disinclinaisons possède un degré élevé de biaxialité, et ne contient pas de liquide isotrope. Enfin, au voisinage des points singuliers en $\mathbb{R}^3$ (défauts de degré 1), une configuration biaxe particulière, nommée « tore biaxe », a été identifiée (voir [51, 81, 82, 132]), bien que son éventuel caractère minimisant ou stable n'ait pas encore été étudié de manière approfondie.

Tous ces résultats n'excluent pas la possibilité que, lorsque $t \gg 1$, les minimiseurs aient un degré de biaxialité très faible partout, à tel point qu'il puissent être considérés comme des petites perturbations d'un état purement uniaxe. Le théorème suivant a pour but d'écarter cette possibilité. À cet effet, il convient d'introduire une quantité qui mesure de façon précise le degré de biaxialité d'un Q-tenseur. Nous utiliserons le *paramètre de biaxialité* défini par

$$\beta(Q) := 1 - 6 \frac{\left(\mathrm{tr}\, Q^3\right)^2}{\left(\mathrm{tr}\, Q^2\right)^3} \qquad \text{pour } 0 \neq Q \in \mathbf{S}_0$$

(voir [103]). Cette quantité satisfait $0 \leq \beta(Q) \leq 1$, avec $\beta(Q) = 0$ si et seulement si Q est uniaxe et $\beta(Q) = 1$ si et seulement si $\det Q = 0$. Elle peut s'écrire en fonction du paramètre r qui apparaît dans la formule de représentation (11).

Nous nous intéressons aux minimiseurs du problème en dimension $N = 2$.

Théorème 1 (C., [29])**.** *Soit $\Omega \subset \mathbb{R}^2$ un domaine borné et régulier, et soit $g \in C^1(\partial\Omega, \mathscr{N})$ une donnée au bord homotopiquement non triviale. Il existe alors $t_0 = t_0(\Omega, g) > 0$ et $\varepsilon_0 = \varepsilon_0(\Omega, g, a, b, c)$ tels que les conditions*

$$t = \frac{ac}{b^2} \geq t_0 \qquad \textit{et} \qquad \varepsilon \leq \varepsilon_0$$

impliquent

$$\min_{\overline{\Omega}} |Q_\varepsilon| > 0 \qquad \textit{et} \qquad \max_{\overline{\Omega}} \beta(Q_\varepsilon) = 1$$

pour tout minimiseur Q_ε de $(\mathrm{LG}_\varepsilon)$ dans la classe $H^1_g(\Omega, \mathbf{S}_0)$.

Lorsque la température est suffisamment basse (et ε est suffisamment petit), le minimiseurs sont biaxes de degré maximum et ne contiennent pas de phases isotropes. Ce dernier fait marque une différence importante avec le modèle d'Ericksen, dans lequel les défauts sont identifiés par la présence de liquide isotrope. L'hypothèse de non-trivialité sur la donnée au bord signifie que g n'est pas prolongeable en une fonction continue $\Omega \to \mathscr{N}$. Cette hypothèse joue un rôle essentiel : dans la section 0.6, on présentera un exemple où la donnée au bord est triviale et les minimiseurs sont purement uniaxes.

Le théorème 1 a été étendu à la dimension $N = 3$ par Contreras et Lamy [35, théorème 1.1], qui montrent aussi l'absence de phases isotropes. Leur preuve, basée sur un argument de blow-up au voisinage des points isotropes, dépend fortement de la condition d'énergie bornée uniformément en ε, (18). En particulier, le théorème de Contreras et Lamy ne s'applique pas en présence de défauts de ligne.

Idée de la preuve du théorème 1

La preuve repose sur un argument purement variationnel. Il suffit de montrer que $\min |Q_\varepsilon| > 0$; comme nous le verrons plus tard, cela entraîne que $\max \beta(Q_\varepsilon) = 1$. Par un changement de variable, minimiser (LG_ε) est équivalent à minimiser la fonctionnelle

$$F_t(Q) := \int_\Omega \left\{ \frac{1}{2} |\nabla Q|^2 + \frac{1}{4\eta^2} \left(1 - |Q|^2\right)^2 + \frac{h(t)}{\eta^2} \varphi(Q) \right\},$$

où le nombre $h(t) > 0$ ne dépend que de t, η est un paramètre dépendant de (ε, t) et φ est un potentiel qui pénalise la biaxialité. Lorsque $t \to +\infty$, nous avons

$$h(t) \sim t^{-1/2}, \quad \frac{1}{\eta^2} \sim t, \qquad \frac{h(t)}{\eta^2} \sim t^{1/2} \tag{23}$$

donc la pénalisation associée à la biaxialité est moins forte que celle associée au module $|Q|$. Pour t suffisamment grand, il est possible de construire une application de comparaison P_t telle que

$$F_t(P_t) \leq \kappa_* \log \eta^{-1} + \frac{\kappa_*}{2} \log h(t) + M,$$

où κ_* est explicitement déterminée et M ne dépend que du domaine et de la donnée au bord. L'étape cruciale de la preuve consiste à obtenir une borne inférieure pour l'énergie : si un minimiseur $Q_t \in C^1(\Omega, \mathbf{S}_0)$ satisfait $\min_\Omega |Q_t| = 0$, alors

$$F_t(Q_t) \geq \kappa_* \log \eta^{-1} - M', \tag{24}$$

pour une autre constante $M' = M'(\Omega, g)$. Puisque (23) implique $\log h(t) \to -\infty$ lorsque $t \to +\infty$, pour t assez grand tout minimiseur Q_t doit satisfaire :

$$F_t(Q_t) \leq F_t(P_t) \leq \kappa_* \log \eta^{-1} + \frac{\kappa_*}{2} \log h(t) + M < \kappa_* \log \eta^{-1} - M',$$

et par contraposition $\min_\Omega |Q_t| > 0$.

Les outils fondamentaux dans la preuve de (24) sont des inégalités démontrées par Jerrard [75, théorème 2.1] et Sandier [123, théorème 1], dans le cadre du modèle de Ginzburg-Landau ; on fait référence ici à l'énoncé de Sandier, qui peut s'exprimer de la façon suivante. Soit $\Omega \subset \mathbb{R}^2$ un domaine simplement connexe, et $D_\varepsilon \subset\subset \Omega$ un sous-domaine de diamètre comparable à ε. Pour toute application $u_\varepsilon \in H^1(\Omega \setminus D_\varepsilon, \mathbb{S}^1)$ il existe une constante C, ne dépendant que de Ω et de $u_{\varepsilon|\partial\Omega}$, telle que

$$\frac{1}{2} \int_{\Omega \setminus D_\varepsilon} |\nabla u_\varepsilon|^2 \geq \pi \left|\deg(u_\varepsilon, \partial\Omega)\right| \log \frac{1}{\varepsilon} - C,$$

où deg désigne le degré topologique. Chiron [33, proposition 6.1] a démontré des estimations analogues, dans le cas où l'application u_ε prend ses valeurs dans le cône sur une variété quelconque $\mathscr{M}$ (défini par (21)). Dans ce cas-ci, $\pi|\deg(u_\varepsilon, \partial\Omega)|$ doit être remplacé par une autre quantité κ_*, qui est fonction de la classe d'homotopie de $u_{\varepsilon|\partial\Omega}$. Lorsque $\mathscr{M} = \mathscr{N} \simeq \mathbb{RP}^2$, la quantité κ_* est la même pour toute application homotopiquement non triviale, et peut être calculée aisément. En s'appuyant sur les arguments de Sandier et sur les propriétés asymptotiques des Q_t, il est possible de prouver (24).

Il reste à voir que $\min_\Omega |Q_t| > 0$ implique $\max_\Omega \beta(Q_t) = 1$; cela repose sur une propriété topologique de l'espace des Q-tenseurs. Nous savons que tout Q-tenseur s'écrit sous la forme

$$Q = s \left(\mathbf{n}^{\otimes 2} - \frac{1}{3} \mathrm{Id} \right) + sr \left(\mathbf{m}^{\otimes 2} - \frac{1}{3} \mathrm{Id} \right),$$

où $\mathbf{n}$, $\mathbf{m}$ sont des vecteurs propres associés aux valeurs propres λ_1, λ_2 (nous rangeons les valeurs propres λ_i de sorte que $\lambda_1 \geq \lambda_2 \geq \lambda_3$). Si $\lambda_1 \neq \lambda_2$, alors $\mathbf{n}$ et $\mathbf{m}$ sont déterminés de façon univoque, au signe près, donc l'application

$$H(Q, t) := s \left(\mathbf{n}^{\otimes 2} - \frac{1}{3} \mathrm{Id} \right) + st \left(\mathbf{m}^{\otimes 2} - \frac{1}{3} \mathrm{Id} \right)$$

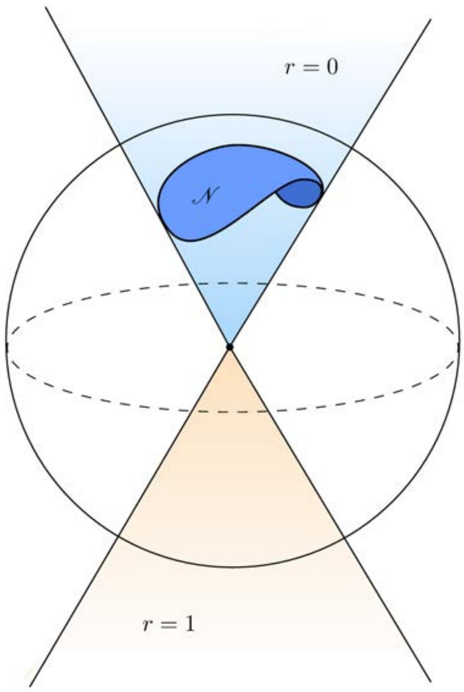


FIGURE 6 – Une représentation symbolique de l'espace des Q-tenseurs. Nous pouvons y reconnaître la sphère unité, les ensembles des matrices uniaxes correspondant à $r = 0$ et $r = 1$ et la variété du vide $\mathscr{N}$, correspondant à l'intersection de la sphère unité avec l'ensemble $\{r = 0\}$.

est bien définie et continue. Puisque $H(Q, 0)$ prend ses valeurs dans la variété $\mathscr{N}$ et que $H(Q, 1)$ est l'identité sur $\mathbf{S}_0$, nous avons construit une rétraction de l'ensemble $\{\lambda_1 \neq \lambda_2\}$ sur $\mathscr{N}$. En utilisant cela, il est facile de voir que toute application continue $Q\colon \Omega \to \mathbf{S}_0$ dont la restriction au bord est une application $\partial\Omega \to \mathscr{N}$ non triviale doit passer par l'ensemble $\{\lambda_1 = \lambda_2\}$, qui est représenté en orange dans la figure 6. En particulier, si $\min_\Omega |Q| > 0$ alors l'image de Q doit passer par les matrices biaxes. Cela explique pourquoi $\max_\Omega \beta(Q_t) = 1$.

5 L'analyse asymptotique des minimiseurs lorsque $\varepsilon \to 0$

5.1 Le cas de la dimension $N = 2$

L'analyse asymptotique des minimiseurs en dimension 2 a été étudiée dans un cadre plus général que celui de la fonctionnelle de Landau-de Gennes (LG_ε). Néanmoins, par souci de simplicité, nous présenterons ici les résultats uniquement dans le cas particulier qui correspond à (LG_ε). On renvoie le lecteur à l'introduction du chapitre 1 pour la description du problème général.

Théorème 2 (C., [29]). *Soit $\Omega \subset \mathbb{R}^2$ un domaine borné et régulier, et soit $g \in C^1(\partial\Omega, \mathscr{N})$ une donnée au bord non triviale. Il existe un point $x_0 \in \Omega$ et une application $Q_0 \in C^\infty(\Omega \setminus \{x_0\}, \mathscr{N})$ tels que, quitte à extraire une sous-suite $\{\varepsilon_n\}_{n\in\mathbb{N}}$ avec $\varepsilon_n \to 0$, nous avons*

$$Q_{\varepsilon_n} \to Q_0 \qquad \text{dans } \left(H^1_{\mathrm{loc}} \cap C^0\right)\left(\overline{\Omega} \setminus \{x_0\}, \mathbf{S}_0\right).$$

L'application Q_0 est localement harmonique minimisante dans $\Omega \setminus \{x_0\}$: en d'autres termes, pour tout *disque $B \subset\subset \Omega \setminus \{x_0\}$ et toute application $P \in H^1(B, \mathbf{S}_0)$,*

$$Q_{0|\partial B} = P_{|\partial B} \qquad \textit{implique} \qquad \frac{1}{2}\int_B |\nabla Q_0|^2 \,\mathrm{d}\mathscr{H}^2 \leq \frac{1}{2}\int_B |\nabla P|^2 \,\mathrm{d}\mathscr{H}^2.$$

En particulier, Q_0 est solution de l'équation des applications harmoniques

$$\Delta Q_0(x) \perp T_{Q_0(x)}\mathscr{N} \qquad \text{pour tout } x \in \Omega \setminus \{x_0\}.$$

Le comportement de Q_0 au voisinage du point singulier x_0 est décrit par le résultat suivant.

Proposition 3 (C., [29]). *À une sous-suite près, la famille de fonctions $c_\rho \colon \mathbb{S}^1 \to \mathscr{N}$ définie par*

$$c_\rho(\omega) := Q_0(x_0 + \rho\omega) \qquad \textit{pour } \omega \in \mathbb{S}^1, \ \rho > 0$$

converge uniformément vers une géodésique de $\mathscr{N}$, de longueur minimale parmi les courbes fermées $\mathbb{S}^1 \to \mathscr{N}$ qui ne sont pas homotopes à une constante.

L'analyse asymptotique de la fonctionnelle (LG_ε) sur des domaines de dimension 2 a été traitée, de façon indépendante, par Golovaty et Montero [55, théorème 1.1]. En utilisant un approche différent (qui est spécifique au problème formulé en termes de Q-tenseurs), ils ont démontré des résultats analogues au théorème 2 et à la proposition 3. De plus, ils caractérisent le comportement de Q_0 au voisinage du point singulier à l'aide d'une application $\psi \colon \Omega \to \mathrm{M}_3(\mathbb{R})$, qui est solution d'un problème elliptique non linéaire [55, théorème 1.2]. Ce dernier résultat est une avancée vers la renormalisation de l'énergie E_ε, qui consiste à écrire un développement de la forme

$$E_\varepsilon(Q_\varepsilon) = \kappa_* \left|\log\varepsilon\right| + W_g(x_0) + c_0 + \mathrm{O}(\varepsilon)$$

où c_0 est une constante et $W_g \colon \Omega \to \mathbb{R}$ est une fonction à déterminer, appelé énergie renormalisée, qui dépend de la donnée au bord. Connaître l'énergie renormalisée permettrait de caractériser la position du point singulier x_0, car on aurait $W_g(x_0) = \inf_\Omega W_g$; au cas contraire, il serait possible de construire des applications P_ε avec une singularité dans un point x_1 tel que $W_g(x_1) < W_g(x_0)$, de sorte que $E_\varepsilon(P_\varepsilon) < E_\varepsilon(Q_\varepsilon)$; cela contredirait la minimalité de Q_ε. La connaissance du comportement local de Q_0 au voisinage de x_0 (et donc la connaissance de la fonction ψ introduite par Golovaty et Montero) devrait nous permettre d'identifier W_g. La notion d'énergie renormalisée a été introduite par Bethuel, Brezis et Hélein [14], en référence à la fonctionnelle de Ginzburg-Landau.

Éléments de la preuve du théorème 2

Cette preuve repose sur un schéma classique, déjà utilisé pour l'analyse asymptotique du problème de Ginzburg-Landau [14, 18, 136]. Tout d'abord, par un argument de comparaison, on établit la majoration logarithmique suivante pour l'énergie :

$$E_\varepsilon(Q_\varepsilon) \leq \kappa_* \left|\log\varepsilon\right| + C \tag{25}$$

où la constante κ_* est optimale. Une fois ce résultat obtenu, nous pouvons passer au coeur de la preuve. Celui-ci réside en une propriété, dite de *nettoyage* (clearing out, en anglais), qui garantit localement l'absence de défauts à condition que l'énergie sur une boule soit suffisamment petite par rapport à $|\log\varepsilon|$. Plus précisément, soient α, $\delta \in (0, 1)$ des paramètres fixés, il existe alors une constante strictement positive $\eta = \eta(\alpha, \delta)$ telle que la condition

$$\int_{B^2(x_0,\, 2\varepsilon^{\alpha/2})\cap\Omega} |\nabla Q_\varepsilon|^2 \,\mathrm{d}\mathscr{H}^2 \leq \eta\left|\log\varepsilon\right| + C$$

implique $\mathrm{dist}(Q_\varepsilon(x), \mathscr{N}) \leq \delta$ pour tout $x \in B^2(x_0, \varepsilon^\alpha) \cap \Omega$. En dimension $N = 2$, cette propriété est une conséquence de l'identité de Pohozaev, appliquée à des boules de rayon ε^α suivant une technique introduite dans [136] et [18]. Une fois que la propriété de nettoyage est prouvée, l'inégalité (25) et un argument de recouvrement permettent de localiser les défauts, c'est-à-dire de montrer que l'ensemble

$$D_\varepsilon := \{x \in \Omega \colon \operatorname{dist}(Q_\varepsilon(x), \mathscr{N}) > \delta\}$$

est contenu dans l'union de K boules de rayon ε^α (où K ne dépend pas de ε). En adaptant les arguments de Bethuel, Brezis et Hélein [14] et de Sandier [123] on voit que, sur un voisinage de l'ensemble singulier

$$D_\varepsilon^\rho := \{x \in \Omega \colon \operatorname{dist}(x, D_\varepsilon) \le \rho\} \qquad \text{avec } \rho > 0,$$

l'énergie est *minorée* par une quantité logarithmique en ε :

$$\int_{D_\varepsilon^\rho} |\nabla Q_\varepsilon|^2 \, \mathrm{d}\mathscr{H}^2 \ge \kappa_* \log \frac{\rho}{\varepsilon} - C.$$

En combinant cette inégalité avec (25), on a

$$\int_{\Omega \setminus D_\varepsilon^\rho} |\nabla Q_\varepsilon|^2 \, \mathrm{d}\mathscr{H}^2 \le C,$$

ce qui entraîne la compacité des minimiseurs. Puisque D_ε est contenu dans l'union de K boules de rayon ε^α, D_ε converge (au sens de la distance de Hausdorff, par exemple) vers un ensemble fini. Enfin, grâce à la structure particulièrement simple du groupe fondamental $\pi_1(\mathscr{N}) \simeq \mathbb{Z}/2\mathbb{Z}$ pour le modèle de Landau-de Gennes, par un argument de comparaison on obtient $D_\varepsilon \to \{x_0\}$.

5.2 Le cas de la dimension $N = 3$

Lorsque la dimension du domaine est $N \ge 3$, les méthodes généralement employées pour l'analyse asymptotique de la fonctionnelle de Ginzburg-Landau ne s'appliquent pas au modèle de Landau-de Gennes pour le régime d'énergie logarithmique (19). En effet, tant les argument de Lin et Rivière [89] pour les minimiseurs que ceux de Bethuel, Brezis et Orlandi [15] pour les points critiques non minimisants font appel à une propriété de nettoyage : pour tout $\delta \in (0, 1)$ il existe une petite constante $\eta > 0$ telle que l'inégalité

$$E_\varepsilon^{\mathrm{GL}}(u_\varepsilon, B_1(x_0)) \le \eta \, |\log \varepsilon| + C \tag{26}$$

(u_ε étant un point critique de $E_\varepsilon^{\mathrm{GL}}$) implique $|u_\varepsilon(x_0)| \ge \delta$, d'où l'absence de défaut. Une propriété de nettoyage avait déjà été utilisée par Bethuel et Rivière [18], dans le cadre de la dimension deux. Dans le travail de Lin et Rivière, le nettoyage est appelé η-compacité ; cependant, malgré le nom, la condition (26) ne suffit *pas* à garantir la compacité des minimiseurs de Ginzburg-Landau (voir la remarque 2). Or, le nettoyage ne peut *pas* être valable pour les minimiseurs de $(\mathrm{LG}_\varepsilon)$ en dimension $N = 3$: en effet, même si l'énergie sur une boule était bornée uniformément en ε, cela n'empêcherait pas la présence de défauts ponctuels.

En dépit du manque de nettoyage, même en dimension $N = 3$ on peut prouver un résultat de compacité pour les minimiseurs de $(\mathrm{LG}_\varepsilon)$, en régime d'énergie logarithmique. Nous considérons ici un domaine borné et lipschitzien $\Omega \subset \mathbb{R}^3$, en imposant des conditions au bord $g_\varepsilon \in H^{1/2}(\partial\Omega, \mathbf{S}_0)$ qui peuvent dépendre de ε. On notera Q_ε un minimiseur de $(\mathrm{LG}_\varepsilon)$ dans la classe $H^1_{g_\varepsilon}(\Omega, \mathbf{S}_0)$.

Théorème 4 (C., [30])**.** *Supposons qu'il existe une constante strictement positive M telle que, pour tout $0 < \varepsilon < 1$,*

$$E_\varepsilon(Q_\varepsilon) \le M \left(|\log \varepsilon| + 1\right) \qquad \text{et} \qquad \|Q_\varepsilon\|_{L^\infty(\Omega)} \le M. \tag{H}$$

Il existe alors une sous-suite $\{\varepsilon_n\}_{n\in\mathbb{N}}$ telle que $\varepsilon_n \searrow 0$, un ensemble relativement fermé $\mathscr{S}_{\mathrm{line}} \subset \Omega$ et une application $Q_0 \in H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathscr{N})$ qui satisfont aux conditions suivantes.

(i) $\mathscr{S}_{\mathrm{line}}$ *est un ensemble* $\mathscr{H}^1$*-rectifiable et* $\mathscr{H}^1(\mathscr{S}_{\mathrm{line}}) < +\infty$.

(ii) Il existe une fonction $\Theta\colon \mathscr{S}_{\mathrm{line}} \to \mathbb{R}^+$*, Borel-mesurable et intégrable par rapport à* $\mathscr{H}^1$*, telle que le couple* $(\mathscr{S}_{\mathrm{line}}, \Theta)$ *définit un varifold stationnaire.*

(iii) $Q_{\varepsilon_n} \to Q_0$ *fortement dans* $H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathscr{N})$.

(iv) Q_0 *est localement harmonique minimisante dans* $\Omega \setminus \mathscr{S}_{\mathrm{line}}$ *: pour toute boule* $B \subset\subset \Omega \setminus \mathscr{S}_{\mathrm{line}}$ *et tout* $P \in H^1(B, \mathscr{N})$*, si* $P_{|\partial B} = Q_{0|\partial B}$ *alors*

$$\frac{1}{2}\int_B |\nabla Q_0|^2 \leq \frac{1}{2}\int_B |\nabla P|^2 .$$

(v) Il existe un ensemble localement fini $\mathscr{S}_{\mathrm{pts}} \subset \Omega \setminus \mathscr{S}_{\mathrm{line}}$ *tel que* Q_0 *est de classe* C^∞ *dans* $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$ *et* $Q_{\varepsilon_n} \to Q_0$ *localement uniformément dans* $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$.

Par définition, l'ensemble $\mathscr{S}_{\mathrm{line}}$ est $\mathscr{H}^1$-rectifiable si et seulement s'il existe une décomposition

$$\mathscr{S}_{\mathrm{line}} = \bigcup_{j \in \mathbb{N}} \mathscr{S}_j ,$$

où $\mathscr{H}^1(\mathscr{S}_0) = 0$ et, pour tout $j \geq 1$, l'ensemble $\mathscr{S}_j$ est l'image d'une fonction lipschitzienne $(0, 1) \to \mathbb{R}^3$. Quant à la notion de varifold stationnaire, elle peut être comprise comme une version faible de variété à courbure moyenne nulle. Contrairement aux variétés lisses, à qui on associe une densité prenant uniquement les valeurs 1 (sur les points de la variété) et 0 (ailleurs), la densité Θ d'un varifold peut prendre des valeurs fractionnaires. Donc les varifold peuvent représenter des « variétés diffusées ». Ce fut Almgren [4] qui introduit cette notion, pour résoudre certains problèmes de calcul des variations ; une contribution importante à la théorie a été donnée par Allard [3]. Le lecteur est renvoyé à [131, chapitres 3, 4] pour une discussion détaillée sur la rectifiabilité et les varifolds stationnaires. Dans notre cas, l'ensemble $\mathscr{S}_{\mathrm{line}}$ et la densité Θ sont définis à partir de la densité d'énergie des minimiseurs, comme nous le verrons par la suite.

Le théorème 4 est de nature locale, et les conditions au bord ne jouent aucun rôle dans la preuve, si ce n'est que d'induire la non-trivialité des minimiseurs. L'application limite Q_0 possède un ensemble de singularités *de ligne* $\mathscr{S}_{\mathrm{line}}$ aussi bien qu'un un ensemble de singularités *ponctuelles* $\mathscr{S}_{\mathrm{pts}}$; cela est en accord avec le résultat de régularité partielle pour les applications harmoniques minimisantes, [125]. Nous donnerons plus tard des exemples où $\mathscr{S}_{\mathrm{line}} \neq \emptyset$. D'autre part, il est facile de construire un exemple où $\mathscr{S}_{\mathrm{pts}} \neq \emptyset$: si Ω contient l'origine et la donnée au bord est définie par

$$g(x) := s_* \left\{ \left(\frac{x}{|x|}\right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right\} \qquad \text{pour } x \in \mathbb{R}^3 \setminus \{0\},$$

alors les résultats de [23, 98] impliquent la convergence $Q_\varepsilon \to g$ dans $H^1(\Omega, \mathbf{S}_0)$. Par conséquent, $\mathscr{S}_{\mathrm{line}} = \emptyset$ mais $\mathscr{S}_{\mathrm{pts}} = \{0\}$. Dans ce cas-ci, la singularité est induite par la donnée au bord non triviale, de degré 1 ; cependant, en dimension 3 des défauts ponctuels pourraient apparaître même en absence d'obstructions topologiques. Ce phénomène a été remarqué par Hardt et Lin [62], pour des applications harmoniques minimisantes. Il est donc possible que l'application Q_0 présente à la fois des singularités de ligne, induites par la topologie, et des singularités ponctuelles non topologiques.

On peut donner des conditions suffisantes, portant sur le domaine et les données au bord, pour que (H) soit satisfaite. La première condition est la suivante.

(H_1) Ω est un domaine borné et régulier, et $\{g_\varepsilon\}_{0<\varepsilon<1}$ est une suite bornée dans $H^{1/2}(\partial\Omega, \mathscr{N})$.

Cette condition est satisfaite lorsque $g_\varepsilon = g$ est régulière à l'exception d'un nombre fini des disinclinaisons, c'est-à-dire de singularités x_0 au voisinages desquelles, en coordonnées polaires géodésiques (ρ, θ) centrées en x_0, g prend la forme

$$g(\rho, \theta) = s_* \left\{ \left(\tau_1 \cos\frac{\theta}{2} + \tau_2 \sin\frac{\theta}{2} \right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right\} + \mathrm{O}(\rho) \qquad \text{pour } \rho \to 0, \tag{27}$$

où (τ_1, τ_2) est un couple orthonormé dans $\mathbb{R}^3$. Nous pouvons également supposer que

(H$_2$) $\Omega \subset \mathbb{R}^3$ est un domaine borné et lipschitzien, et il existe un homéomorphisme bi-lipschitzien de Ω dans un corps à anses (c'est-à-dire, une boule attachée à un nombre fini d'anses).

(H$_3$) Il existe $M_0 > 0$ tel que, pour tout $0 < \varepsilon < 1$, on a $g_\varepsilon \in (H^1 \cap L^\infty)(\partial\Omega, \mathbf{S}_0)$ et

$$E_\varepsilon(g_\varepsilon, \partial\Omega) \leq M_0\left(|\log\varepsilon| + 1\right), \qquad \|g_\varepsilon\|_{L^\infty(\partial\Omega)} \leq M_0.$$

La condition (H$_3$) est satisfaite si les fonctions g_ε sont des approximations régulières d'une application g de la forme (27) ; on pourra prendre par exemple

$$g_\varepsilon(\rho, \theta) := \eta_\varepsilon(\rho) g(\rho, \theta) \tag{28}$$

où $\eta_\varepsilon \in C^\infty(0, +\infty)$ satisfait

$$\eta_\varepsilon(0) = \eta_\varepsilon'(0) = 0, \qquad \eta_\varepsilon(\rho) = 1 \text{ si } \rho \geq \varepsilon, \qquad 0 \leq \eta_\varepsilon \leq 1, \qquad |\eta_\varepsilon'| \leq C\varepsilon^{-1}.$$

Proposition 5 (C., [30]). *Si la condition* (H$_1$) *est satisfaite, ou bien si* (H$_2$)–(H$_3$) *sont satisfaites, alors* (H) *est satisfaite aussi.*

En prenant des conditions au bord de la forme (28), il est possible d'induire des singularités de ligne dans la limite $\varepsilon \to 0$, sur n'importe quel domaine. Plus précisément, nous avons ce résultat :

Proposition 6 (C., [30]). *Pour tout domaine borné $\Omega \subset \mathbb{R}^3$ de classe C^1, il existe une famille $\{g_\varepsilon\}_{0<\varepsilon<1}$ satisfaisant* (H$_3$) *et un nombre $\alpha > 0$ tel que*

$$E_\varepsilon(Q) \geq \alpha\left(|\log\varepsilon| - 1\right)$$

pour tout $Q \in H^1_{g_\varepsilon}(\Omega, \mathbf{S}_0)$ et $0 < \varepsilon < 1$. En particulier, aucune sous-suite de minimiseurs ne converge dans $H^1(\Omega, \mathbf{S}_0)$.

Éléments de la preuve du théorème 4

L'ingrédient fondamental de la preuve est fourni par la proposition suivante.

Proposition 7 (C., [30]). *Supposons la condition* (H) *satisfaite. Pour tout $0 < \theta < 1$, il existe des constantes strictement positives η, ϵ_0 et C avec la propriété suivante. Pour tout point $x_0 \in \Omega$, tout rayon $R > 0$ tel que $B_R(x_0) \subset\subset \Omega$ et tout $0 < \varepsilon \leq \epsilon_0 R$, si la condition*

$$E_\varepsilon(Q_\varepsilon, B_R(x_0)) \leq \eta R \log\frac{R}{\varepsilon} \tag{29}$$

est vérifiée, alors

$$E_\varepsilon(Q_\varepsilon, B_{\theta R}(x_0)) \leq CR.$$

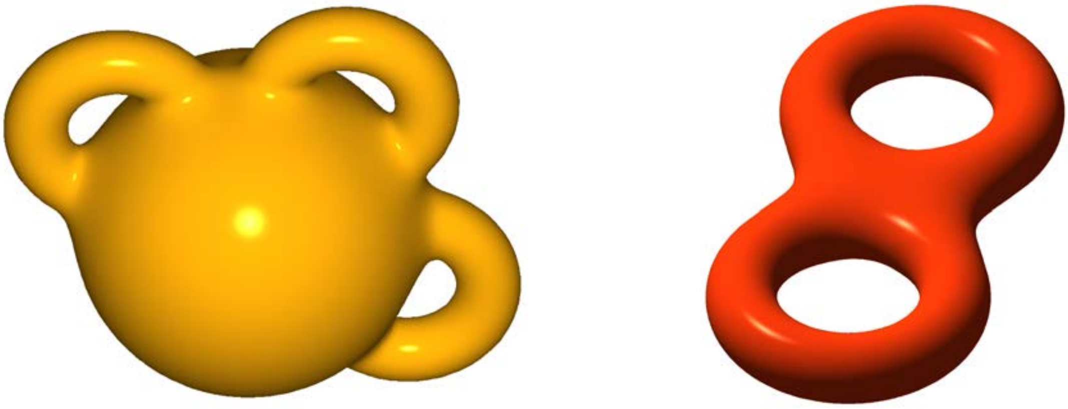


Figure 7 – À gauche, une sphère à trois anses ; à droite, un tore à deux trous. Ces deux domaines satisfont la condition (H_2). Remarquons que le bord de tout domaine satisfaisant (H_2) est connexe.

En supposant cette propriété acquise, nous définissons les mesures positives $(\mu_\varepsilon)_{0<\varepsilon<1}$ par

$$\mu_\varepsilon(B) := \frac{E_\varepsilon(Q_\varepsilon,\, B)}{|\log\varepsilon|} \qquad \text{pour } B \in \mathscr{B}(\Omega).$$

Grâce à la condition (H), la famille des variations totales de ces mesures est uniformément bornée ; donc, quitte à extraire une sous-suite $\varepsilon_n \searrow 0$, nous avons la convergence faible au sens des mesures bornées :

$$\mu_{\varepsilon_n} \rightharpoonup^* \mu_0 \qquad \text{faiblement}^* \text{ dans } \mathscr{M}_{\mathrm{b}}(\Omega) := C_0(\Omega)'.$$

En passant à la limite dans la proposition 7, nous déduisons que

$$\mu_0\left(\overline{B}_R(x_0)\right) < \eta R \qquad \text{implique} \qquad \mu_0\left(B_{R/2}(x_0)\right) = 0,$$

ou encore que

$$\Theta(x_0) := \liminf_{R\to 0} \frac{\mu_0(\overline{B}_R(x_0))}{2R} \geq \frac{\eta}{2} \qquad \mu_0\text{-p.p. en } x_0. \tag{30}$$

Cette propriété fournit, par des arguments de recouvrement classiques (voir [131, théorème 3.2]), que le support $\mathscr{S}_{\mathrm{line}}$ de μ_0 est de dimension de Hausdorff inférieure ou égale à 1. La rectifiabilité de $\mathscr{S}_{\mathrm{line}}$ en découle aussi, grâce à un théorème de Preiss (voir [115, théorème 5.3] ou [39, théorème 1.1]). De plus, la proposition 7 implique que l'énergie des minimiseurs est bornée uniformément en ε sur tout ensemble $K \subset\subset \Omega \setminus \mathscr{S}_{\mathrm{line}}$, d'où la compacité faible des Q_ε dans $H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}},\, \mathbf{S}_0)$. La compacité forte et le caractère harmonique minimisant de l'application limite se démontrent par des variantes d'arguments classiques, comme ceux de Majumdar et Zarnescu [98]. Enfin, par les techniques de Ambrosio et Soner [6, section 3] on prouve que $(\mathscr{S}_{\mathrm{line}},\, \Theta)$ définit un varifold stationnaire.

Nous évoquons ici les idée principales de la preuve de la proposition 7, d'un point de vue heuristique. En premier lieu, on établit des estimations d'énergie analogues à celles de Jerrard [75] et Sandier [123] : sous des hypothèses techniques adéquates, si la restriction au bord d'une application $Q \in W^{1,\infty}(B^2_1,\, \mathbf{S}_0)$ est homotopiquement non triviale, alors

$$E_\varepsilon(Q,\, B^2_1) \geq \kappa_* \log\frac{1}{\varepsilon} - C \tag{31}$$

pour une constante $\kappa_* > 0$ dépendant seulement de f. Grâce à ce résultat, on peut voir que l'hypothèse (29) exclut la présence de ligne de défauts topologiques, si η est suffisamment petit. En effet, (29) implique, par argument de moyenne,

$$E_\varepsilon(Q_\varepsilon,\, \partial B_r(x_0)) \leq \eta' \log\frac{r}{\varepsilon} \tag{32}$$

pour un ensemble de rayons $r \in (\theta R,\, R)$ de mesure suffisamment grande et une constante $\eta' \propto \eta$. Cette inégalité contredit (31) lorsque η' est suffisamment petit ; par conséquent, la classe d'homotopie de Q_ε le long de toute courbe fermée contenue dans $\partial B_r(x_0)$ est triviale. Grâce à cette propriété topologique, nous pouvons approcher Q_ε avec une application continue $P_\varepsilon \colon \partial B_r(x_0) \to \mathscr{N}$, dont l'énergie est contrôlée par celle de Q_ε. Puisque la sphère $\partial B_r(x_0)$ est simplement connexe, la fonction P_ε admet un relèvement lisse $\mathbf{n}_\varepsilon \colon \partial B_r(x_0) \to \mathbb{S}^2$. En d'autres termes, nous pouvons écrire

$$Q_\varepsilon(x) \simeq P_\varepsilon(x) = s_* \left(\mathbf{n}_\varepsilon^{\otimes 2}(x) - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{pour } x \in \partial B_r(x_0). \tag{33}$$

Cela réduit le problème à l'analyse des applications à valeurs dans $\mathbb{S}^2$, pour lesquelles il est possible d'utiliser les méthodes de Hardt, Kinderlehrer et Lin [60]. En particulier, en prolongeant $\mathbf{n}_\varepsilon$ à l'intérieur de $B_r(x_0)$ de manière opportune (comme dans [60, lemme 2.3]) et par un argument de comparaison, nous obtenons

$$E_\varepsilon(Q_\varepsilon,\, B_r(x_0)) \leq Cr E_\varepsilon^{1/2}(Q_\varepsilon,\, \partial B_r(x_0)) + R \tag{34}$$

pour tout $r \in (\theta R,\, R)$ satisfaisant l'inégalité (32). En introduisant la fonction $h_\varepsilon(r) := E_\varepsilon(Q_\varepsilon, B_r(x_0)) - R$, cette inégalité peut s'écrire sous la forme

$$h_\varepsilon^2(r) \leq Cr^2 h_\varepsilon'(r) \tag{35}$$

pour tout r satisfaisant (32). Supposons ici, par souci de simplicité, que (35) soit satisfaite pour tout $r \in (\theta R,\, R)$. Cette inégalité différentielle peut s'intégrer de façon explicite, et nous obtenons

$$h_\varepsilon(r) \geq \frac{\alpha_\varepsilon \theta C R\, r}{(\theta C R - \alpha_\varepsilon) r + \alpha_\varepsilon \theta R}$$

où $\alpha_\varepsilon := h_\varepsilon(\theta R)$. En particulier, l'intervalle d'existence maximale $[\theta R,\, \rho_\varepsilon)$ pour une solution de (35) vérifie

$$\rho_\varepsilon \leq \frac{\alpha_\varepsilon \theta R}{\alpha_\varepsilon - \theta C R}.$$

D'autre part, il est clair que $\rho_\varepsilon \geq R$, car h_ε est définie sur $(\theta R,\, R]$ au moins. En combinant ces inégalités, nous déduisons que

$$\alpha_\varepsilon \leq \frac{\theta C R}{1 - \theta},$$

c'est-à-dire que l'énergie $E_\varepsilon(Q_\varepsilon,\, B_{\theta R}(x_0))$ ne peut pas dépasser un certain seuil.

En quelques mots, l'idée de la preuve de la proposition 7 pourrait être résumée ainsi : lorsque l'énergie est petite par rapport à $|\log \varepsilon|$, il n'y a pas d'obstructions topologiques engendrées par $\pi_1(\mathscr{N})$; alors, par relèvement, l'analyse des minimiseurs de $(\mathrm{LG}_\varepsilon)$ peut être ramenée à l'analyse des minimiseurs de l'énergie d'Oseen-Frank.

Revenons sur un point technique, mais d'importance cruciale, qui intervient dans la preuve de (34). Cette inégalité est obtenue par un argument de comparaison : nous voulons comparer l'énergie du minimiseur Q_ε sur la boule $B_r(x_0)$ avec l'énergie d'une autre application convenablement choisie. Pour que cela soit possible, il faut que les deux applications coïncident sur la sphère $\partial B_r(x_0)$. Cela nous amène à construire une application φ_ε, définie sur une couronne de largeur suffisamment petite, telle que $\varphi_\varepsilon = Q_\varepsilon$ sur le bord extérieur de la couronne et $\varphi_\varepsilon = P_\varepsilon$ sur le bord intérieur, où P_ε est l'application approchée qui apparaît dans l'équation (33). La construction de φ_ε repose sur une technique introduite par Luckhaus [92, lemme 1] et illustrée dans la figure 8. Nous considérons une grille sur la sphère $\partial B_r(x_0)$ avec des propriétés adéquates. Ensuite, nous définissons φ_ε par interpolation linéaire sur le bord des mailles de la grille, et nous l'étendons à l'intérieur des mailles par des extensions homogènes. Néanmoins, il y a deux différences par rapport au résultat de Luckhaus. En premier lieu, dans le lemme de Luckhaus les deux applications Q_ε et P_ε sont données, alors qu'ici seulement Q_ε est donnée et P_ε est à déterminer en fonction de Q_ε. Deuxièmement, il faut garantir une estimation non seulement sur le gradient de φ_ε, mais aussi sur le terme d'énergie potentielle $\varepsilon^{-2} f(\varphi_\varepsilon)$; cela est possible pour un choix adéquat de P_ε. La section 2.3.2 du chapitre 2 est consacrée à la discussion de ce point.

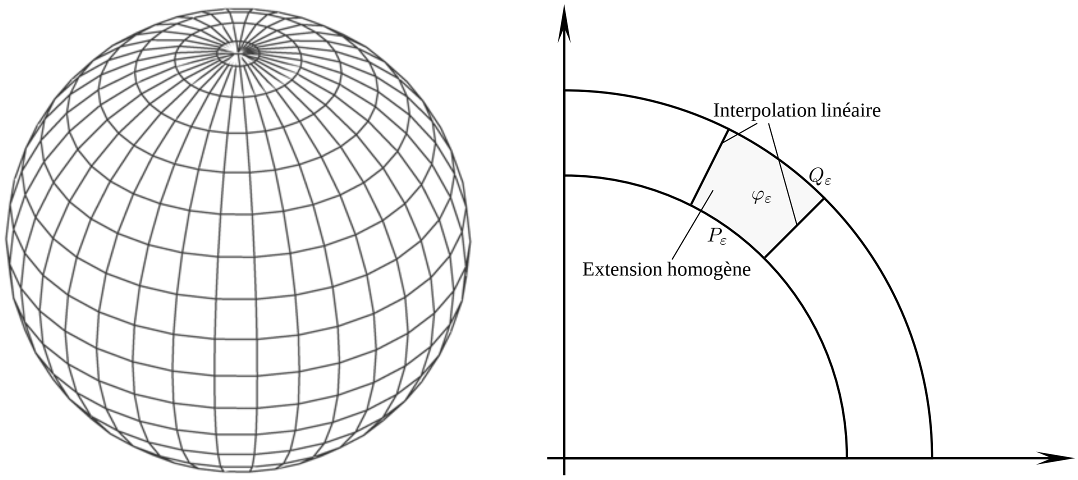


FIGURE 8 – À gauche, une grille sur la sphère. À droite, une représentation schématique de la construction de Luckhaus. Soient données deux applications Q_ε, P_ε, définies sur le bord extérieur et intérieur d'une couronne. On construit φ_ε par interpolation linéaire sur le bord des mailles de la grille ; on l'étend à l'intérieur des mailles par des extensions homogènes.

Remarque 2. D'après le théorème 4, l'hypothèse (H) implique la compacité des minimiseurs de $(\mathrm{LG}_\varepsilon)$. Cela constitue une différence importante avec le modèle de Ginzburg-Landau, où la seule condition (H) ne garantit pas de compacité pour les minimiseurs. En effet, Brezis et Mironescu [24] ont construit une suite de minimiseurs $u_{\varepsilon_n} \in H^1(B_1^2, \mathbb{C})$ satisfaisant

$$E^{\mathrm{GL}}_{\varepsilon_n}(u_{\varepsilon_n}, B_1^2) \ll |\log \varepsilon_n| \qquad \text{et} \qquad |u_{\varepsilon_n}| \leq 1,$$

bien que $\{u_{\varepsilon_n}\}$ n'admet aucune sous-suite convergeant p.p. sur aucun ensemble de mesure strictement positive. Pour cette suite, les données au bord $g_n := u_{\varepsilon_n | \partial B_1^2}$ sont des fonctions très oscillantes, car

$$g_n(x) = e^{inx_1} \qquad \text{pour tout } x \in \partial B_1^2 \text{ et tout } n.$$

En particulier, la suite des relèvements $\partial B_1^2 \to \mathbb{R}$ (c'est-à-dire, $x \mapsto inx_1$) n'est *pas* bornée dans $L^\infty(\partial B_1^2)$. Ce contre-exemple repose sur le fait que, pour la fonctionnelle de Ginzburg-Landau, la variété du vide $\mathbb{S}^1$ possède un recouvrement universel *non compact*. Par contre, dans le cas de Landau-de Gennes, le recouvrement universel de $\mathscr{N}$ est la variété compacte $\mathbb{S}^2$. Par conséquent, la compacité du recouvrement universel (qui dépend de la finitude du groupe fondamental) semblerait être liée à des meilleures propriétés de compacité pour les minimiseurs.

6 La limite des basses températures sur une couronne dans $\mathbb{R}^3$

La limite $\varepsilon \to 0$ n'est pas le seul régime asymptotique intéressant pour la fonctionnelle $(\mathrm{LG}_\varepsilon)$. Une autre possibilité est d'étudier le problème, à constante élastique $\varepsilon > 0$ fixée, lorsque la température tend vers $-\infty$. Bien entendu, si la température est très basse le matériau n'est plus en phase nématique, mais en phase solide ; donc, le modèle de Landau-de Gennes perd sa validité physique. Néanmoins, l'étude asymptotique pour les basses températures permet parfois d'apporter des éclairages sur certains problèmes d'intérêt physique. Les travaux de Henao et Majumdar [71] et Contreras et Lamy [35] en sont des exemples : dans les deux cas, des propriétés de biaxialité des minimiseurs sont démontrées en faisant appel à l'analyse asymptotique pour les basses températures. Les arguments présentés dans la section 0.4 vont aussi dans cette direction.

Pour l'étude mathématique du problème, il convient de mettre en évidence le paramètre t, défini par (22), qui est proportionnel à la température au signe près. À cet effet, nous effectuons un changement de variables, en définissant

$$\tilde{Q} := \frac{1}{s_*}\sqrt{\frac{3}{2}}Q \;;$$

nous supposons aussi que

$$\varepsilon = \frac{b}{2\sqrt{2c}},$$

car cela permet de simplifier certaines constantes. Puisque, de toute façon, ε était supposé fixé et strictement positif, cette hypothèse ne compromet pas la généralité du discours. En fonction de la nouvelle variable, la fonctionnelle prend la forme

$$(\mathrm{LG}_t) \qquad F_t(Q) := \int_\Omega \left\{ \frac{1}{2}\left|\nabla Q\right|^2 + \frac{t}{8}\left(1 - |Q|^2\right)^2 + \frac{\lambda(t)}{8}\left(1 - 4\sqrt{6}\,\mathrm{tr}\, Q^3 + 3|Q|^4\right) \right\}$$

où les tildes ont été omis, par souci de simplicité ; la constante $\lambda(t)$ est donnée par

$$\lambda(t) := \frac{\sqrt{24t+1}+1}{36}.$$

La fonctionnelle (LG_t) présente une caractéristique spécifique par rapport à $(\mathrm{LG}_\varepsilon)$, à savoir, elle contient deux termes de pénalisation d'ordres différents en t. Le premier terme est associé à un potentiel de type Ginzburg-Landau, portant sur le module de Q, avec une pénalisation linéaire en t. La biaxialité n'est pénalisée qu'à travers le second terme, avec un coefficient moins fort, homogène à $t^{1/2}$ lorsque $t \to +\infty$.

Dans un travail en collaboration avec Apala Majumdar et Mythily Ramaswamy [97], nous avons considéré la fonctionnelle (LG_t) sur une couronne $\Omega := B_R(0) \setminus \overline{B}_1(0) \subset \mathbb{R}^3$, pour $R > 1$. En imposant des conditions au bord à symétrie radiale, de la forme

$$(36) \qquad Q(x) = H_\infty(x) := \left(\frac{x}{|x|}\right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \qquad \text{pour } x \in \partial\Omega,$$

on calcule facilement (grâce à [72, lemme A.1]) qu'il existe un seul point critique de (LG_t) à symétrie radiale, satisfaisant ces conditions au bord. Cette configuration, appelée *hérisson uniaxe*, est donnée par

$$H_t(x) := h_t(|x|)\left\{\left(\frac{x}{|x|}\right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right\} \qquad \text{pour } x \in \Omega,$$

où la fonction $h_t \colon [1,\, R] \to \mathbb{R}$ est déterminée en tant que solution du problème

$$(37) \qquad \begin{cases} h_t'' + \dfrac{2}{\rho}h_t' - \dfrac{6}{\rho^2}h_t = \dfrac{t}{2}h_t\left(h_t^2 - 1\right)^2 + \dfrac{3\lambda(t)}{2}\left(h_t^3 - h_t^2\right) & \text{sur } (1,\, R) \\ h_t(1) = h_t(R) = 1. \end{cases}$$

En fait le hérisson uniaxe est le seul point critique de (LG_t) dans la classe des configurations purement uniaxes (c'est-à-dire, $Q \colon \Omega \to \mathbf{S}_0$ telles que $\beta(Q) = 0$ sur tout le domaine). Cela est un résultat de Lamy [83] ; la preuve de ce théorème a été donnée lorsque le domaine est une boule, mais elle demeure valable sur une couronne aussi. Le résultat suivant (qui, par ailleurs, est indépendant du théorème de Lamy) donne des conditions suffisantes pour que le hérisson uniaxe soit minimiseur.

Théorème 8 (Majumdar, C., Ramaswamy, [97]). *Soit $\mathscr{A}$ la classe des configurations $Q \in H^1(\Omega, \mathbf{S}_0)$ qui satisfont la condition au bord* (36)*, au sens des traces. Il existe un nombre strictement positif $R_0 > 0$ et une fonction $\tau \colon [0,\, +\infty) \to [0,\, +\infty)$ tels que, si l'une des conditions*

$$\text{(i)} \quad R - 1 \leq R_0 \qquad \textit{ou bien} \qquad \text{(ii)} \quad t \geq \tau(R-1)$$

est satisfaite, alors H_t est le seul minimiseur de (LG_t) *dans $\mathscr{A}$.*

En d'autres termes, le hérisson uniaxe est le seul minimiseur (par rapport à sa propre condition au bord) pour toute température si la largeur de la couronne est petite, ou bien si la température est basse, pour n'importe quelle valeur de $R - 1$. De plus, en utilisant l'équation (37), il est possible de voir que $h_t \to 1$ uniformément sur $[1, R]$, lorsque $t \to +\infty$. Il en découle comme corollaire que les minimiseurs de (LG_t) convergent uniformément vers l'application harmonique minimisante H_∞, lorsque $t \to +\infty$ (le caractère minimisant de H_∞ est une conséquence du résultat de Brezis, Coron et Lieb [23, théorème 7.1]). Ce théorème donne aussi un exemple de minimiseur uniaxe, dans le régime des basses températures. Cela ne contredit pas le théorème 1 ni [35, théorème 1.1], car la donnée au bord $H_{\infty|\partial\Omega}$ est topologiquement triviale.

La preuve du théorème est basée sur une analyse attentive des différents termes dans l'énergie. Dans les deux cas, la preuve comprend trois étapes : démontrer la stabilité du hérisson uniaxe, c'est-à-dire prouver que la variation second de l'énergie est positive ; montrer que $|h_t| \simeq 1$ en appliquant le principe du maximum à l'équation (37) ; borner par dessous les termes d'order supérieur, grâce aux informations sur la partie quadratique de l'énergie et sur $|h_t|$. Pour démontrer la stabilité du hérisson, on utilise dans le cas (i) une inégalité de type Hardy. Dans le cas (ii), on applique les méthodes de [73], où la stabilité du hérisson est prouvée pour un régime de température différent, dans l'espace $\mathbb{R}^3$.

7 La formule de l'indice de Morse pour des champs de vecteurs dans VMO

Dans cette section, on présente des résultats obtenus en collaboration avec Antonio Segatti et Marco Veneroni, portant sur une obstruction topologique à l'existence de champs de vecteurs unitaires de faible régularité. Ce travail a été motivé par une question qui se pose naturellement lorsqu'on veut étudier des modèles variationnels pour des cristaux liquides étalés sur une surface $\mathscr{M} \subset \mathbb{R}^d$. Dans le cas le plus simple possible, la configuration est représentée par un champ de vecteurs unitaires $\mathbf{v}$ défini sur $\mathscr{M}$ et l'énergie associée se réduit à la fonctionnelle de Dirichlet (2). Supposons que $\mathscr{M}$ est une surface à bord, et imposons des conditions au bord de Dirichlet. Nous voulons caractériser les données au bord $\mathbf{g}\colon \partial\mathscr{M} \to \mathbb{S}^{d-1}$ prolongeables à des champs de vecteurs unitaires dans l'espace d'énergie, c'est-à-dire l'espace de Sobolev $W^{1,2}(\mathscr{M}, \mathbb{R}^d)$.

La réponse à cette question dépendra des propriétés topologiques de la surface $\mathscr{M}$. Par exemple, dans le cas $\mathscr{M} = \mathbb{S}^2$ l'existence de champs de vecteurs unitaires réguliers est interdite par le Théorème de la boule chevelue. Plus généralement, l'existence de champs de vecteurs unitaires réguliers sur une variété obéit à une obstruction topologique.

Soit $\mathscr{M} \subset \mathbb{R}^d$ une variété avec ou sans bord, de dimension $2 \leq m < d$, lisse, compacte, connexe et orientable. Soit $\mathbf{v}\colon \mathscr{M} \to \mathbb{S}^d$ un champ de vecteurs unitaires continu. Supposons que

$$\mathbf{v}(x) \neq 0 \qquad \text{pour tout } x \in \partial\mathscr{M} \tag{38}$$

et que $\mathbf{v}$ ne s'annule qu'en un nombre fini de points $x_1, x_2, \ldots, x_p \in \mathscr{M} \setminus \partial\mathscr{M}$. Pour chaque x_i il est possible de définir un nombre entier, appelé *indice local* ou *degré local*, qui décrit le comportement du champ au voisinage de x_i. Les indices locales se définissent à l'aide du degré topologique : en identifiant $\mathbf{v}$ à une application $\mathbb{R}^m \to \mathbb{R}^m$, par composition avec cartes locales, et en prenant une petite boule géodésique $B_r(x_i)$ qui ne contient aucun $x_j \neq x_i$, nous posons

$$\mathrm{ind}(\mathbf{v},\, x_i) := \deg\left(\frac{\mathbf{v}}{|\mathbf{v}|},\, \partial B_r(x_i),\, \mathbb{S}^{m-1}\right).$$

Il est facile de voir que le membre de gauche ne dépend pas du choix des cartes locales, ni de la boule (à condition qu'elle ne contienne pas de zéros de $\mathbf{v}$ autres que x_i). L'*indice* de $\mathbf{v}$ sera alors défini par

$$\mathrm{ind}(\mathbf{v},\, \mathscr{M}) := \sum_{i=1}^{p} \mathrm{ind}(\mathbf{v},\, x_i).$$

Pour tenir compte du comportement de $\mathbf{v}$ au bord, nous introduisons aussi l'*indice au bord entrant* :

$$\mathrm{ind}_-(\mathbf{v},\, \partial\mathscr{M}) := \mathrm{ind}(P_{\partial\mathscr{M}}\mathbf{v},\, \partial_-\mathscr{M}[\mathbf{v}])$$

où $\partial_-\mathscr{M}[\mathbf{v}]$ est le sous-ensemble du bord sur lequel $\mathbf{v}$ pointe vers l'intérieur de $\mathscr{M}$, et $P_{\partial\mathscr{M}}\mathbf{v}$ est la composante tangente au bord :

$$P_{\partial\mathscr{M}}\mathbf{v}(x) := \mathrm{proj}_{T_x\partial\mathscr{M}}\mathbf{v}(x) \qquad \text{pour tout } x \in \partial\mathscr{M}.$$

Si $\partial_-\mathscr{M}[\mathbf{v}] = \emptyset$, nous posons $\mathrm{ind}_-(\mathbf{v},\, \partial\mathscr{M}) := 0$. L'indice au bord entrant est bien défini à condition que $P_{\partial\mathscr{M}}\mathbf{v}$ ait un nombre fini de zéros. Nous avons alors le résultat (classique) suivant :

Théorème 9 (Formule de l'indice de Morse, [106])**.** *Soit* $\mathbf{v}$ *un champ de vecteurs continu sur* $\mathscr{M}$*, satisfaisant* (38)*, avec un nombre fini de zéros. Si la projection* $P_{\partial N}\mathbf{v}$ *a un nombre fini de zéros, alors*

$$\mathrm{ind}(\mathbf{v},\, \mathscr{M}) + \mathrm{ind}_-(\mathbf{v},\, \mathscr{M}) = \chi(\mathscr{M}), \tag{39}$$

où $\chi(\mathscr{M})$ *est la caractéristique d'Euler-Poincaré de* $\mathscr{M}$*.*

Ce résultat généralise un théorème célèbre, dit de Poincaré-Hopf, qui traite le cas où $\partial_-M[\mathbf{v}] = \emptyset$ (voir [101, chapitre 6] pour une preuve de ce dernier). À son tour, la formule de Morse a été redécouverte et généralisée par Pugh [116] et Gottlieb [56, 57]. Grâce à ce théorème, on peut voir aisément qu'une fonction continue $\mathbf{g}\colon \partial\mathscr{M} \to \mathbb{S}^{d-1}$ satisfaisant $\mathbf{g}(x) \in T_x\mathscr{M}$ pour tout $x \in \partial\mathscr{M}$ est prolongeable à un champ de vecteurs unitaires continu si et seulement si

$$\mathrm{ind}_-(\mathbf{g},\, \partial\mathscr{M}) = \chi(\mathscr{M}). \tag{40}$$

D'autre part, ce théorème n'est pas applicable aux fonctions de régularité Sobolev. La définition d'indice elle-même, étant basée sur les valeurs ponctuelles de $\mathbf{v}$, ne s'étend pas directement aux fonctions Sobolev. Pour contourner cette difficulté, il convient de reformuler le problème dans le cadre fonctionnel $\mathrm{VMO}(\mathscr{M},\, \mathbb{R}^d)$. Cet espace, introduit par Sarason [124], est une variante de l'espace BMO de John et Nirenberg [77]. Il peut être défini comme le complété des fonctions continues $C^0(\mathscr{M}, \mathbb{R}^d)$ par rapport à la norme

$$\|\mathbf{u}\|_{\mathrm{BMO}} := \sup_{x,\, \varepsilon} \fint_{B_\varepsilon^{\mathscr{M}}(x)} |\mathbf{u} - \bar{\mathbf{u}}_\varepsilon(x)| \,\mathrm{d}\mathscr{H}^m,$$

où le supremum est pris sur tous les $\varepsilon > 0$ et tous les $x \in \mathscr{M}$ tels que $\mathrm{dist}(x,\ ,\partial\mathscr{M}) > 2\varepsilon$, et

$$\bar{\mathbf{u}}_\varepsilon(x) := \fint_{B_\varepsilon^{\mathscr{M}}(x)} \mathbf{u} \,\mathrm{d}\mathscr{H}^m.$$

De manière équivalente, une fonction $\mathbf{u} \in L^1(\mathscr{M},\, \mathbb{R}^d)$ appartient à $\mathrm{VMO}(\mathscr{M},\, \mathbb{R}^d)$ si et seulement si

$$\lim_{\varepsilon\to 0} \sup_{x\in\mathscr{M}} \fint_{B_\varepsilon^{\mathscr{M}}(x)} |\mathbf{u} - \bar{\mathbf{u}}_\varepsilon(x)| \,\mathrm{d}\mathscr{H}^m = 0.$$

Puisque les fonctions $x \mapsto \mathbf{u}_\varepsilon(x)$ sont continues, pour tout ε fixé, cette caractérisation donne une manière canonique d'approcher une fonction donnée $\mathbf{u} \in \mathrm{VMO}(\mathscr{M},\, \mathbb{R}^d)$ par des applications continues. En utilisant cela, Brezis et Nirenberg [25, 26] ont développé une théorie du degré topologique pour fonctions VMO. Des généralisations de la notion de degré pour fonctions non continues avaient déjà été données dans plusieurs cas (voir, par exemple, [21, 22]) ; la théorie de Brezis et Nirenberg donne un cadre général qui permet un traitement unifié de ce cas particuliers. La théorie dans VMO s'applique aussi aux fonctions Sobolev, grâce à l'inclusion continue

$$W^{s,p}(\mathscr{M},\, \mathbb{R}^d) \hookrightarrow \mathrm{VMO}(\mathscr{M},\, \mathbb{R}^d) \qquad \text{pour } sp = m$$

qui fait intervenir les espaces critiques par rapport aux inclusions de Sobolev.

Inspirés par les travaux de Brezis et Nirenberg, nous avons voulu généraliser la théorie de l'indice, définie au départ pour les champs de vecteurs continus ayant un nombre fini de zéros, aux champs VMO. Comme étape préliminaire, nous nous sommes intéressés au cas des fonctions continues satisfaisant (38) et s'annulant sur un ensemble de cardinal infini ; ce cas a été traité par une application du théorème de transversalité de Thom [137, 138], un outil très puissant de géométrie différentielle. Nous avons ensuite traité le problème dans le cadre VMO, en raisonnant essentiellement par densité. La difficulté principale, ici, est le manque d'un opérateur de trace au bord : par exemple, la fonction $x \mapsto \cos(\log|\log x|)$ appartient à $H^{1/2}(0, 1/2) \subset \mathrm{VMO}(0, 1/2)$ mais sa trace au point $x = 0$ n'est pas définie. Cependant, comme montré par Brezis et Nirenberg [26], il existe une sous-classe dans VMO pour laquelle il est possible de définir la trace au bord ; il s'agit d'une notion de trace bien particulière car elle n'est pas stable par rapport à la convergence dans VMO. Néanmoins elle répond à nos besoins. Grâce à ces outils, il a été possible de démontrer le résultat suivant.

Théorème 10 (C., Segatti, Veneroni, [31])**.** *Soit $\mathscr{M} \subset \mathbb{R}^d$ une variété lisse à bord, compacte, connexe et orientable. Supposons que $\mathbf{g} \in \mathrm{VMO}(\partial\mathscr{M}, \mathbb{R}^d)$ satisfait*

$$\mathbf{g}(x) \in T_x\mathscr{M} \qquad \text{et} \qquad c_1 \leq |\mathbf{g}(x)| \leq c_2$$

p.p. en $x \in \partial\mathscr{M}$, pour deux constantes strictement positives c_1, c_2. Si $\mathbf{v} \in \mathrm{VMO}(\mathscr{M}, \mathbb{R}^d)$ admet $\mathbf{g}$ comme trace au bord, au sens de Brezis et Nirenberg, et si $\mathbf{v}(x) \in T_x\mathscr{M}$ p.p. en $x \in \mathscr{M}$, alors (39) est satisfaite. De plus, la condition (40) est nécessaire et suffisante pour qu'il existe un champ $\mathbf{v} \in \mathrm{VMO}(\mathscr{M}, \mathbb{R}^d)$ de trace $\mathbf{g}$, tel que

$$\mathbf{v}(x) \in T_x\mathscr{M} \qquad \text{et} \qquad c_1 \leq |\mathbf{v}(x)| \leq c_2 \qquad \text{p.p en } x \in \mathscr{M}.$$

Dans le cas où les données au bord appartiennent à un espace Sobolev de trace, c'est-à-dire $\mathbf{g} \in W^{1-1/p,p}(\partial\mathscr{M}, \mathbb{R}^d)$ avec $1 < p < +\infty$, alors le prolongement $\mathbf{v}$ peut être choisi de sorte que $\mathbf{v} \in W^{1,p}(\mathscr{M}, \mathbb{R}^d)$.

Pour finir, revenons à l'interprétation en termes de nématiques étalés sur une surface. En raison de la symétrie $\mathbf{n} \leftrightarrow -\mathbf{n}$ qui caractérise le vecteur directeur du nématique, on pourrait objecter que les champs de vecteurs (orientés) ne sont pas très adéquats à représenter les matériaux nématiques, et qu'il serait plus approprié d'utiliser de *champs de lignes non orientées*. Pour cette raison, dans la dernière partie de ce travail nous définissons la notion de champ de lignes VMO, en utilisant le formalisme des Q-tenseurs, et nous nous intéressons aux obstructions topologiques à l'existence de tels objets. Dans le cas des variétés sans bord, nous démontrons la même obstruction que pour les champs de vecteurs unitaires continus, à savoir, un champ de lignes VMO existe si et seulement si $\chi(\mathscr{M}) = 0$. Le cas des variétés à bord comporte une difficulté supplémentaire, qui n'est pas de nature analytique mais topologique : existe-t-il un équivalent de la formule de l'indice de Morse pour les champs de lignes réguliers ? En particulier, la définition de l'indice au bord sortant pourrait être problématique, en l'absence d'orientation. Ces difficultés pourraient être contournées en faisant appel à des outils de topologie différentielle (en particulier, le recouvrement orienté d'une foliation ; voir, par exemple, [65]), qui permettraient de se ramener à l'étude des champs orientés. Cependant, dans le travail présent nous n'avons pas traité ce point, qui pourra être l'objet d'un développement futur.

8 Conclusions et perspectives

En résumé, le sujet principal de cette thèse concerne les minimiseurs de la fonctionnelle de Landau-de Gennes (LG_ε), sous l'approximation à une constante pour l'énergie élastique, en l'absence de champs électromagnétiques extérieurs. Deux questions notamment ont été traitées :

- ◇ le comportement asymptotique des minimiseurs pour $\varepsilon \to 0$. En particulier, on s'intéresse au cas où l'énergie des minimiseurs satisfait une borne logarithmique, en étudiant la convergence vers des applications localement harmoniques ayant des singularités de codimension deux, dans un domaine de dimension 2 ou 3 ;

- ◇ la présence de phases biaxes dans le noyau des singularités, lorsque la température est suffisamment basse (en dimension 2).

Plusieurs questions restent ouvertes, notamment dans le cas tridimensionnel.

Structure de l'ensemble singulier pour l'analyse asymptotique en dimension 3

Comme nous avons vu dans la sous-section 0.5.2, sous l'hypothèse (H) il existe un ensemble relativement fermé $\mathscr{S}_{\mathrm{line}} \subset \Omega$ tel que la suite des minimiseurs de $(\mathrm{LG}_\varepsilon)$ soit compacte dans $H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathbf{S}_0)$. L'ensemble $\mathscr{S}_{\mathrm{line}}$ est défini comme le support d'une mesure μ_0 qui est point d'accumulation faible-$*$ de la suite

$$\mu_\varepsilon := \left\{ \frac{1}{2} \left|\nabla Q_\varepsilon\right|^2 + \frac{1}{\varepsilon^2} f(Q_\varepsilon) \right\} \frac{\mathrm{d}x}{|\log \varepsilon|} \in \mathscr{M}_{\mathrm{b}}(\Omega).$$

On montre ensuite que $\mathscr{S}_{\mathrm{line}}$ est 1-rectifiable, et qu'il est un varifold stationnaire. Malheureusement, cela ne donne pas beaucoup d'informations sur la régularité de $\mathscr{S}_{\mathrm{line}}$. En effet, le principal résultat de régularité pour les varifold stationnaires — le théorème d'Allard, [3, théorème 5.5] — ne s'applique que lorsque la densité de $\mathscr{S}_{\mathrm{line}}$ (la fonction Θ définie par (30)) prend ses valeurs dans un ensemble discret. En vue de l'estimation de type Jerrard-Sandier (31), on pourrait s'attendre à ce que

$$\Theta(x) = \kappa_* \qquad \mathscr{H}^1\text{-p.p. en } x \in \mathscr{S}_{\mathrm{line}},$$

où κ_* est la constante qui apparaît dans (31). (L'inégalité $\geq$ serait une conséquence de (31), alors que $\leq$ devrait faire intervenir la minimalité de Q_ε). Par le théorème d'Allard, cela impliquerait que $\mathscr{S}_{\mathrm{line}} = \mathscr{S}_0 \cup \mathscr{S}_1$, où $\mathscr{H}^1(\mathscr{S}_0) = 0$ et $\mathscr{S}_1$ est une courbe lisse. Ensuite, grâce à la stationnarité de $\mathscr{S}_{\mathrm{line}}$, on obtiendrait que $\mathscr{S}_1$ est une union de segments de droite, connectant entre elles les singularités de la donnée au bord. Dans des cas simples au moins, on peut s'attendre à ce qu'il n'y ait pas de points de branchement (de telles configurations de lignes singulières seraient moins favorables, en termes de longueur, par rapport à d'autres configurations sans branchements). Ainsi, $\mathscr{S}_{\mathrm{line}}$ pourrait se réduire à une union de lignes droites.

Les difficultés techniques qui se profilent dans cette direction dépendent du fait que la structure de $\mathscr{S}_{\mathrm{line}}$ pourrait être très complexe. Par exemple, $\mathscr{S}_{\mathrm{line}}$ pourrait contenir une infinité de composantes connexes, qui se rassemblent au voisinage d'un point. Cela rend plus délicate la mise en oeuvre des arguments de comparaison.

Comportement des minimiseurs au voisinage de l'ensemble singulier

Si l'on dispose d'informations supplémentaires sur la régularité de $\mathscr{S}_{\mathrm{line}}$ (en particulier, s'il s'avère que $\mathscr{S}_{\mathrm{line}}$ est une union de lignes droites), alors il peut être intéressant d'étudier plus en détail le comportement des minimiseurs dans le noyau des défauts de ligne. Par exemple, on pourrait étudier le problème de minimisation sur un voisinage tubulaire de la singularité, avec des données au bord qui prennent leurs valeurs près de la variété du vide $\mathscr{N}$. Compte tenu des résultats de la section 0.4, on pourrait conjecturer que les minimiseurs présentent des phases biaxes dans le noyau des défauts.

Une question connexe est l'étude des *profils de singularité* associés aux singularités de ligne. Soit $x_0 \in \mathscr{S}_{\mathrm{line}}$, et soit Π un plan orthogonal à $\mathscr{S}_{\mathrm{line}}$ au point x_0. Les fonctions définies par

$$P_{\varepsilon, x_0}(y) := Q_\varepsilon(x_0 + \varepsilon y) \qquad \text{pour } y \in \Pi$$

sont bornées dans $L^\infty(\Pi, \mathbf{S}_0)$ et satisfont à

$$\|\nabla P_{\varepsilon, x_0}\|_{L^2(K)} = \|\nabla Q_\varepsilon\|_{L^2(x_0 + \varepsilon K)} \leq C(K) \qquad \text{pour tout } K \subset\subset \Pi,$$

donc $P_{\varepsilon, x_0} \rightharpoonup P_{x_0}$ dans $H^1_{\mathrm{loc}}(\Pi, \mathbf{S}_0)$, à une sous-suite près. Qu'est-ce qu'on peut dire de l'application P_{x_0}, qui contient les informations sur la structure fine de la singularité ? Dans des cas simples (par exemple, si la donnée au bord sur toute coupe transversale à $\mathscr{S}_{\text{line}}$ est la même), on pourrait s'attendre à ce que le profil P_{x_0} soit indépendant du choix de x_0, et qu'il soit complètement déterminé par le problème de minimisation en dimension 2. La situation devrait être plus compliquée pour les minimiseurs de l'énergie à quatre constantes élastiques (13), puisque les minimiseurs de l'énergie d'Oseen-Frank (1) dans un cylindre dépendent de la variable parallèle à l'axe du cylindre (voir [122]).

Étude de la Γ-convergence de la fonctionnelle renormalisée

Par analogie avec des résultats connus sur la fonctionnelle de Ginzburg-Landau [2, 76], on pourrait conjecturer la Γ-convergence

$$I_\varepsilon := \frac{E_\varepsilon}{|\log \varepsilon|} \to I_0,$$

où I_0 est une fonctionnelle définie sur un espace de courants de dimension 1, exprimant la longueur des lignes de défaut (pondérée par une quantité qui prend en compte la charge topologique). La difficulté principale consiste à déterminer la topologie dans laquelle la Γ-convergence a lieu.

Analyse asymptotique de fonctionnelles plus générales

Enfin, il serait intéressant d'étudier le comportement asymptotique de fonctionnelles plus générales, incluant par exemple plusieurs constantes élastiques, ou bien utilisant des potentiels différents de (16). Des potentiels intéressants du point de vue physique sont, par exemple, le potentiel de Landau-de Gennes de degré six

$$f(Q) := -\frac{a_1}{2}\operatorname{tr} Q^2 - \frac{a_2}{3}\operatorname{tr} Q^3 + \frac{a_3}{4}\left(\operatorname{tr} Q^2\right)^2 + \frac{a_4}{5}\left(\operatorname{tr} Q^2\right)\left(\operatorname{tr} Q^3\right) + \frac{a_5}{6}\left(\operatorname{tr} Q^2\right)^3 + \frac{a_5'}{6}\left(\operatorname{tr} Q^3\right)^2$$

(voir, par exemple, [36, 58]) ou le potentiel singulier proposé par Ball et Majumdar [9]. L'analyse du problème sous sa forme la plus générale possible (en particulier, avec une constante élastique $L_4 \neq 0$) demande probablement des techniques nouvelles par rapport à celles développées dans cette thèse. Toutefois, on peut espérer que les méthodes utilisées dans la preuve de la proposition 7 puissent être adaptées à des cas intérmediaires (par exemple, le cas $L_4 = 0$).

Plan de la thèse

Ce manuscrit s'organise de la manière suivante. Dans le chapitre 1, on s'intéresse au problème dans un domaine en dimension 2. La biaxialité des minimiseurs (voir la section 0.4) et l'analyse asymptotique lorsque $\varepsilon \to 0$ (sous-section 0.5.1) y sont traitées. Le chapitre 2 porte sur l'analyse asymptotique des minimiseurs en dimension 3. La limite des basses températures sur une couronne est détaillée dans le chapitre 3. Enfin, le chapitre 4 est consacré à la formule de l'indice de Morse pour les champs de vecteurs VMO.

General introduction

1 The Landau-de Gennes model for liquid crystals

1.1 Classification of Q-tensors

Liquid crystals are matter in an intermediate phase between liquid and crystalline solid states. They are composed by molecules which can flow freely but tend to arrange in an ordered way. As a result, liquid crystals can form droplets and are unable to support shear, as a conventional liquid. On the other hand, they are anisotropic with respect to optical and electromagnetic properties, which makes them suitable for many applications. Liquid crystals phases (which are also known as *mesophases*) can be divided into several classes. Throughout this thesis, we will consider only *nematic* liquid crystals. In this phase, the centers of mass of molecules are distributed randomly but the axes of the molecules tend to align locally, along some preferred directions. Moreover, we assume that the material is composed by *uniaxial* molecules, i.e. molecules with an axis of rotational symmetry, for instance rod-shaped molecules.

Different continuum theories have been proposed to model uniaxial nematic liquid crystals. Among them, the Landau-de Gennes theory or Q-tensor theory allows a rather complete description of the local behaviour of the medium. The arrangement of molecules at a given point is described by a real 3×3 symmetric traceless matrix $Q = Q(x)$, depending on the position x. Such a matrix can be interpreted as the renormalized second order moment of the orientation distribution function of molecules. States are classified according to the eigenvalues of Q.

- $Q = 0$ corresponds to an *isotropic* phase, i.e. completely lacking of orientational order.
- Matrices $Q \neq 0$ with two identical eigenvalues are said to be *uniaxial*. They represent configurations with an axis of rotational symmetry. In particular, a unique preferred direction of molecular alignment is defined.
- Matrices Q with distinct eigenvalues are called *biaxial*. The corresponding states lack of rotational symmetry, but have three orthogonal axes of reflection symmetry. More preferred directions of molecular alignments exist.

The adjectives “uniaxial” and “biaxial” here refer to the *arrangement* of molecules, not to the molecules themselves which are assumed to be uniaxial. (For more details about uniaxial and biaxial arrangements, the reader might consult [108]). Every Q-tensor can be represented as follows:

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) + sr\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) \tag{1}$$

where $s \geq 0$, $0 \leq r \leq 1$ and $(\mathbf{n},\, \mathbf{m})$ is a positively oriented orthonormal pair in $\mathbb{R}^3$. The parameters s and r are uniquely determined by Q. The number s measures the degree of order of the configuration, whereas r is related to biaxiality. In particular, a matrix Q is uniaxial if and only if $r \in \{0,\, 1\}$. When $r = 1$, the identity $\mathrm{Id} = \mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2} + \mathbf{m}^{\otimes 2}$ (for $\mathbf{p} := \mathbf{n} \times \mathbf{m}$) gives

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) + s\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) = -s\left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right).$$

The vectors $\mathbf{n}$ and $\mathbf{m}$ describe the orientation of the symmetry axes of the local configuration.

1.2 The variational problem

Let $\mathbf{S}_0 \simeq \mathbb{R}^5$ be the space of 3×3, real symmetric traceless matrices. The order parameter is a function $Q\colon \Omega \to \mathbf{S}_0$, where $\Omega \subseteq \mathbb{R}^N$ is a bounded smooth domain, $N \in \{2, 3\}$. The stable configurations are minimizers of the Landau-de Gennes energy

$$E_\varepsilon(Q) := \int_\Omega \left\{\frac{1}{2}\left|\nabla Q\right|^2 + \frac{1}{\varepsilon^2} f(Q)\right\}, \tag{LG$_\varepsilon$}$$

subject to the (ε-independent) Dirichlet boundary condition

$$Q_\varepsilon = g \qquad \text{on } \partial\Omega \text{ in the sense of traces.} \tag{2}$$

The potential f is given by

$$f(Q) := -\frac{a}{2}\,\mathrm{tr}\, Q^2 - \frac{b}{3}\,\mathrm{tr}\, Q^3 + \frac{c}{4}\left(\mathrm{tr}\, Q^2\right)^2. \tag{3}$$

The positive parameters a, b and c depend on the material and the temperature, and ε^2 is a material-dependent elastic constant, typically very small (of the order of 10^{-11} Jm^{-1}). The function f is bounded from below, and the set

$$\mathscr{N} := \{Q \in \mathbf{S}_0 \colon f(Q) = \min f\}$$

is a smooth manifold, called the *vacuum manifold*, diffeomorphic to the real projective plane $\mathbb{RP}^2$ (see [98, Proposition 9]). In terms of the representation formula (1), the vacuum manifold can be characterized as follows:

$$Q \in \mathscr{N} \qquad \text{if and only if} \qquad s(Q) = s_*,\ r(Q) = 0,$$

where s_* is the positive constant given by

$$s_* = s_*(a,\, b,\, c) := \frac{b + \sqrt{b^2 + 24ac}}{4c}.$$

In particular, the elements of $\mathscr{N}$ are all uniaxial matrices.

Let us discuss some heuristic ideas on this problem. When ε is small, any minimizer Q_ε of (LG$_\varepsilon$) is forced to take its values as close as possible to the vacuum manifold $\mathscr{N}$. However, since the topology of $\mathscr{N}$ is non-trivial, continuous maps $\Omega \to \mathscr{N}$ satisfying the boundary condition may not exist. Boundary data for which this obstruction occurs will be referred to as non-trivial. Thus, as $\varepsilon \to 0$ we expect that minimizers converge to $\mathscr{N}$-valued maps with singularities, called *defects*, which are characteristic features of the experimental observations. Far from the defect core, minimizers take values close to the vacuum manifold, therefore they consist of uniaxial (or approximately uniaxial) states. However, the defect core can contain isotropic or biaxial phases.

The setting of the problem changes substantially, depending on the dimension N of the domain. When $N = 2$, there is no map in $H^1(\Omega,\, \mathscr{N})$ which satisfies the Dirichlet conditions (2), unless the boundary datum is trivial (see [14]). If the boundary datum is a smooth map $\partial\Omega \to \mathscr{N}$, then minimizers satisfy the energy estimate

$$E_\varepsilon(Q_\varepsilon) \leq \kappa_* \left|\log \varepsilon\right| + C \tag{4}$$

for some constant $\kappa_* = \kappa_*(a, b, c) > 0$. This estimate is sharp. Indeed, if the boundary datum is non-trivial then minimizers also satisfy the lower bound

$$E_\varepsilon(Q_\varepsilon) \geq \kappa_* \left|\log \varepsilon\right| - C' \tag{5}$$

(analogous bounds have been previously obtained by Jerrard [75, Theorem 2.1] and Sandier [123, Theorem 1]). In the limit as $\varepsilon \to 0$, minimizers converge to a map with point defects, whose behaviour is controlled by the first homotopy group $\pi_1(\mathscr{N})$. In contrast, when $N = 3$ both point and line defects are possible, so topological obstructions to the regularity may occur from $\pi_1(\mathscr{N})$ and $\pi_2(\mathscr{N})$. As we will see, line defects are associated with a logarithmic growth of the energy as in (4), but point singularities might exist even where the energy is bounded.

The functional (LG$_\varepsilon$) bears some similarities to the Ginzburg-Landau energy, given by

$$E_\varepsilon^{\mathrm{GL}}(u) := \int_\Omega \left\{ \frac{1}{2} \left|\nabla u\right|^2 + \frac{1}{4\varepsilon^2} \left(1 - |u|^2\right)^2 \right\} \tag{6}$$

where $u \colon \Omega \to \mathbb{C}$ (we are neglecting the electromagnetic field here). For this model, the formation of topological singularities is a well-understood mechanism (the reader is referred to [14, 18, 136] for the case $N = 2$ and to [15, 89] for $N \geq 3$). A logarithmic energy bound such as (4) has been proven to be involved in the formation of codimension two topological singularities. In the case $N = 2$, it is worth mentioning the estimates by Jerrard [75] and Sandier [123], which provide a lower bound for the energy of a map $u \colon \Omega \to \mathbb{C}$, i.e.

$$E_\varepsilon^{\mathrm{GL}}(u) \geq \pi \left|\deg(u, \partial\Omega)\right| \left|\log \varepsilon\right| - C$$

for $\deg(u, \partial\Omega)$ is the topological degree of u at the boundary. This estimate has a counterpart in the Landau-de Gennes model, namely (5). (Note that, in the Landau-the Gennes model, the fundamental group $\pi_1(\mathscr{N}) = \pi_1(\mathbb{RP}^2)$ has just two elements, so all the non-trivial boundary data belongs to the same homotopy class. This is why the constant κ_* which appears in (5) is the same for every non-trivial datum.) For each $N \geq 2$, a Γ-convergence result

$$I_\varepsilon(u) := |\log \varepsilon|^{-1} E_\varepsilon^{\mathrm{GL}}(u) \to I_0(u) \qquad \text{as } \varepsilon \to 0$$

has been proved (see [2, 76]). Here I_0 is a functional defined on the space of $(N-2)$-currents, proportional to the $(N-2)$-measure of the defects, weighted by some quantity which accounts for their topological properties. Therefore, codimension 2 defects are associated with the logarithmic energy regime.

Despite the similarity between the Ginzburg-Landau energy (6) and (LG$_\varepsilon$), there are also important differences between the two models. For instance, the set of minimizers for $u \mapsto (1 - |u|^2)^2$ is the unit circle $\mathbb{S}^1$, which has codimension one in $\mathbb{C}$, whereas $\mathscr{N}$ has codimension three in $\mathbf{S}_0$. In particular, a minimizer of (6) is forced to take the value 0 near a singularity, whereas several behaviours are possible for minimizers of (LG$_\varepsilon$), and isotropic points (i.e. $Q = 0$) can be avoided by a "biaxial escape".

2 Mathematical analysis of the Landau-de Gennes model

2.1 The analysis of a two-dimensional case

In Chapter 1, we study minimizers of (LG$_\varepsilon$) when $N = 2$. Two main questions are addressed:

- For a small $\varepsilon > 0$, how does Q_ε behave near the defects? Are there biaxial or isotropic points?
- Do minimizers Q_ε converge as $\varepsilon \to 0$? In which sense?

When studying the possible biaxiality of minimizers, one should take into account the temperature [93, 112]. The temperature T is involved in the minimization problem through the potential f. More precisely, one has

$$t := \frac{ac}{b^2} \propto T_0 - T, \tag{7}$$

where T_0 is the temperature at which isotropic-nematic transition occurs. In the following, we always assume that $T < T_0$ so that $t > 0$. There is numerical evidence that biaxiality should be expected in the core of defects (see [128]). Results implying the biaxiality of minimizers for $t \gg 1$ have already been proved. The unique radially symmetric uniaxial critical point — the so-called *radial-hedgehog* — becomes unstable if t is large (see [51] and [73, Theorem 1.2]). Henao and Majumdar [71, Theorem 1] and, later, Lamy [83, Theorems 4.1 and 5.1] proved that minimizers on a three-dimensional domain cannot be purely uniaxial if $t \gg 1$. Lamy also proved that, in a two-dimensional domain, critical points cannot be purely uniaxial if the boundary datum is non-trivial. However, all these results do not exclude "almost uniaxial" minimizers, i.e. configurations with such a small degree of biaxiality to be physically indistinguishable from uniaxial ones. The biaxiality of a matrix Q is measured by the parameter

$$\beta(Q) := 1 - 6\frac{\left(\operatorname{tr} Q^3\right)^2}{\left(\operatorname{tr} Q^2\right)^3},$$

ranging from 0 to 1, with $\beta(Q) = 0$ if and only if Q is uniaxial. Our first goal is to rule out this possibility.

Theorem 1 (C., [29]). *Assume that the boundary datum is a smooth, non-trivial map $\partial\Omega \to \mathscr{N}$. There exist $t_0 = t_0(\Omega, g) > 0$ and $\varepsilon_0 = \varepsilon_0(\Omega, g, a, b, c)$ such that the conditions*

$$\frac{ac}{b^2} \geq t_0 \qquad \text{and} \qquad \varepsilon \leq \varepsilon_0$$

imply

$$\min_{\overline{\Omega}} |Q_\varepsilon| > 0, \qquad \max_{\overline{\Omega}} \beta(Q_\varepsilon) = 1$$

for any minimizer Q_ε of (LG_ε).

Thus, when the temperature is low, the core of defects is highly biaxial with no isotropic point. In contrast, other popular models for liquid crystals (e.g. the Ericksen model) predict isotropic phases in the core of defects. The proof of Theorem 1 relies on a variational argument. With the help of the coarea formula and the results of [123], the energy of any uniaxial configuration is bounded from below. Then, one constructs a biaxial competitor with energy smaller than this bound, and conclude that minimizers must be biaxial.

As for the asymptotic analysis, we have the following result.

Theorem 2 (C., [29]). *Assume that the boundary datum is a smooth, non-trivial function $\partial\Omega \to \mathscr{N}$. There exists a point $x_0 \in \Omega$, a map $Q_0 \in C^\infty(\Omega \setminus \{x_0\}, \mathscr{N})$ and a subsequence $\varepsilon_n \to 0$ such that*

$$Q_{\varepsilon_n} \to Q_0 \qquad \text{in } \left(H^1_{\mathrm{loc}} \cap C^0\right)(\Omega \setminus \{x_0\}, \mathbf{S}_0).$$

The map Q_0 is locally minimizing harmonic on $\Omega \setminus \{x_0\}$, that is for every ball $B \subseteq \Omega \setminus \{x_0\}$ and any $P \in H^1(B, \mathbf{S}_0)$ such that $Q_{0|\partial B} = P_{|\partial B}$ we have

$$\frac{1}{2}\int_B |\nabla Q_0|^2 \leq \frac{1}{2}\int_B |\nabla P|^2 .$$

Moreover, the functions $c_\rho \colon \mathbb{S}^1 \to \mathscr{N}$ defined by

$$c_\rho(\omega) := Q_0(x_0 + \rho\omega) \qquad \text{for } \omega \in \mathbb{S}^1$$

converge uniformly to a geodesic in $\mathscr{N}$, up to a subsequence.

Theorem 2 is recovered as a particular case of a more general result, where $\mathscr{N}$ is assumed to be a smooth, compact, connected manifold, and $f \geq 0$ is a smooth potential with a non-degenerate behaviour around $\mathscr{N}$. The singular set of Q_0 is finite, and it reduces to a single point when $\mathscr{N} \simeq \mathbb{RP}^2$. The proof is based on the strategy of [14, 18]. Combining a clearing-out property, local Pohozaev identities and Jerrard-Sandier type estimates [75, 123], one shows that the energy diverges logarithmically on a finite number of small balls, and is bounded elsewhere. A convergence result in the same spirit has been obtained independently by Golovaty and Montero [55, Theorem 1.1], with a different approach.

2.2 A convergence result on three-dimensional domains

In case Ω is a bounded, Lipschitz domain of dimension $N = 3$ and the energy of minimizers satisfies a uniform bound, then minimizers of $(\mathrm{LG}_\varepsilon)$ converge strongly in H^1 as $\varepsilon \to 0$. The limiting map has isolated point singularities, and actually we have locally uniform convergence away from the singularities (this was proved by Majumdar and Zarnescu [98, Propositions 5 and 7]). However, if we assume that the energy of minimizers satisfies a logarithmic bound such as (4), then the picture is different. Line singularities can appear in the limit, in addition to point singularities. For the following results, the boundary data $g_\varepsilon \in H^{1/2}(\partial\Omega, \mathbf{S}_0)$ are allowed to depend on ε.

Theorem 3 (C., [30])**.** *Assume that there exists a positive constant M such that, for any $0 < \varepsilon < 1$, there holds*

$$E_\varepsilon(Q_\varepsilon) \leq M\left(|\log\varepsilon| + 1\right) \qquad \text{and} \qquad \|Q_\varepsilon\|_{L^\infty(\Omega)} \leq M. \tag{H}$$

Then, there exist a subsequence $\varepsilon_n \searrow 0$, a relatively closed set $\mathscr{S}_{\mathrm{line}} \subseteq \Omega$ and a map $Q_0 \in H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathscr{N})$ such that the following holds.

(i) $\mathscr{S}_{\mathrm{line}}$ is a countably $\mathscr{H}^1$-rectifiable set, and $\mathscr{H}^1(\mathscr{S}_{\mathrm{line}}) < +\infty$.

(ii) There exists a positive, Borel function $\Theta\colon \mathscr{S}_{\mathrm{line}} \to \mathbb{R}^+$ such that $(\mathscr{S}_{\mathrm{line}}, \Theta)$ defines a stationary varifold.

(iii) $Q_{\varepsilon_n} \to Q_0$ strongly in $H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathscr{N})$.

(iv) Q_0 is locally minimizing harmonic in $\Omega \setminus \mathscr{S}_{\mathrm{line}}$.

(v) There exists a locally finite set $\mathscr{S}_{\mathrm{pts}} \subseteq \Omega \setminus \mathscr{S}_{\mathrm{line}}$ such that Q_0 is smooth on $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$ and $Q_\varepsilon \to Q_0$ locally uniformly in $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$.

The rectifiability condition means that $\mathscr{S}_{\mathrm{line}}$ is smooth in a measure-theoretical sense. Theorem 3 also implies that $\mathscr{S}_{\mathrm{line}}$ can be given a structure of stationary varifold. Stationary varifolds are a weak version of minimal manifolds, introduced by Almgreen [4] to deal with variational problems. They have a density Θ which, in the smooth case, reduces to a $\{0, 1\}$-valued function ($\Theta = 1$ on the manifold, and $\Theta = 0$ elsewhere). In general, Θ may take real values, so varifolds can be understood as a sort of "diffuse manifolds". The reader is referred to e.g. [131, Chapters 3 and 4] for a detailed discussions on rectifiable sets and varifolds. In our case, $\mathscr{S}_{\mathrm{line}}$ is defined as the support of the measure μ_0, which is a weak* limit of the energy densities:

$$\left\{\frac{1}{2}\left|\nabla Q_{\varepsilon_n}\right|^2 + \frac{1}{{\varepsilon_n}^2} f(Q_{\varepsilon_n})\right\} \mathrm{d}x \rightharpoonup^* \mu_0 \qquad \text{in } C_0(\Omega)'.$$

The density Θ is also defined in terms of μ_0:

$$\Theta(x) := \lim_{r\to 0^+} \frac{\mu_0(\overline{B}_r(x))}{2r} \qquad \text{for all } x \in \mathscr{S}_{\mathrm{line}}$$

(it can be proved that the function $r \mapsto (2r)^{-1}\mu_0(\overline{B}_r(x))$ is monotone, so the limit exists for all x).

We provide some sufficient conditions on Ω and the boundary datum which ensure that the condition (H) is satisfied. For instance, one can assume that the domain is smooth and $\{g_\varepsilon\}_{0<\varepsilon<1}$ is a bounded sequence in $H^{1/2}(\Omega, \mathscr{N})$. Condition (H) also holds if we assume that $g_\varepsilon \in H^1(\Omega, \mathbf{S}_0)$ satisfies

$$E_\varepsilon(g_\varepsilon, \partial\Omega) \leq M_0 \left(|\log\varepsilon| + 1\right), \qquad \|g_\varepsilon\|_{L^\infty(\partial\Omega)} \leq M_0$$

for any $0 < \varepsilon < 1$, together with a topological condition on Ω. To construct examples of boundary data which satisfy these assumptions, we consider maps $\partial\Omega \to \mathscr{N}$ with a finite number of point singularities, or smooth approximations of such maps.

The key point in the proof of Theorem 3 is a concentration result for the energy. Given $0 < \theta < 1$, there exist positive numbers ε_0 η and C such that, for any $0 < \varepsilon \leq \varepsilon_0$, the condition

$$E_\varepsilon(Q_\varepsilon, B_1(x_0)) \leq \eta\,|\log\varepsilon| \tag{8}$$

implies

$$E_\varepsilon(Q_\varepsilon, B_\theta(x_0)) \leq C. \tag{9}$$

As a result, the energy of minimizers is locally bounded away from the support of the limit measure μ_0. This provides compactness of minimizers. Then, the properties of $\mathscr{S}_{\mathrm{line}}$ can be studied by measure-theoretical arguments. Heuristically speaking, the proof of (9) can be summarized as follows. The assumption (8), for η small enough, implies that Q_ε has no topological singularity on a small sphere $\partial B_r(x_0)$, for $\theta < r < 1$. Then, by lifting, the problem can be reduced to the analysis of $\mathbb{S}^2$-valued maps. Indeed, one can write

$$Q_\varepsilon(x) \simeq s_*\left(\mathbf{n}_\varepsilon^{\otimes 2}(x) - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{for } x \in \partial B_r(x_0),$$

where $\mathbf{n}_\varepsilon$ is a smooth $\mathbb{S}^2$-valued map. Therefore, it is possible to deal with the problem by using the methods introduced by Hardt, Kinderlehrer and Lin [60] in the analysis of the Oseen-Franck model. Several tools are exploited in the proof, including Jerrard-Sandier type estimates [75, 123], the “hybrid inequality” by Hardt, Kinderlehrer and Lin [60, Lemma 2.3], and a variant of Luckhaus' interpolation lemma [92, Lemma 1].

2.3 The low-temperature limit on spherical shells

We also consider a different asymptotic problem for the Landau-de Gennes functional, namely, we fix the elastic constant ε and let the temperature tend to $-\infty$. Of course, if the temperature is low enough then the nematic phase loses stability, and the material enters the solid state. However, the asymptotic analysis of this limit is an interesting mathematical problem, and it can be used to derive meaningful conclusions on situations of clear physical interest (e.g. as in [35, 71]).

By changing the variable of (LG_ε), we are led to consider the functional

$$F_t(Q) := \int_\Omega \left\{\frac{1}{2}\,|\nabla Q|^2 + \frac{t}{8}\left(1 - |Q|^2\right)^2 + \frac{\lambda(t)}{8}\left(1 - 4\sqrt{6}\,\mathrm{tr}\,Q^3 + 3|Q|^4\right)\right\} \tag{LG_t}$$

where t is the parameter defined by (7), which is proportional to the opposite of the temperature. We are interested in the limit as $t \to -\infty$. Here $\lambda(t)$ is a quantity depending on t, such that $\lambda(t) \sim Ct^{1/2}$ as $t \to -\infty$. Compared to (LG_ε), the functional (LG_t) has an additional difficulty, since there are two terms of different orders in t. In Chapter 3, which reports on a joint work with Majumdar and Ramaswamy, we consider (LG_t) on a spherical shell $\Omega := B_R(0) \setminus \overline{B}_1(0) \subseteq \mathbb{R}^3$. We study the so-called *radial-hedgehog*:

$$H_t(x) := h_t(|x|)\left\{\left(\frac{x}{|x|}\right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right\} \qquad \text{for every } x \in \Omega,$$

where h_t is the characterized as a solution of an ODE, with $h_t(1) = h_t(R) = 1$. Note that the boundary datum $H_{t|\partial\Omega}$ is independent of t. The radial-hedgehog is the unique uniaxial, radially symmetric critical point for (LG_t) (see [73, Lemma A.1]), and the natural candidate to be a minimizer.

Theorem 4 (Majumdar, C. and Ramaswamy, [97]). *Let* $\mathscr{A} := \left\{Q \in H^1(\Omega, \mathbf{S}_0) \colon Q_{|\partial\Omega} = H_{t|\partial\Omega}\right\}$ *be the class of admissible configurations. There exist a positive number* R_0 *and a function* $\tau \colon [0, +\infty) \to [0, +\infty)$ *such that, if either*

$$\text{(i)} \quad R - 1 \leq R_0 \qquad \textit{or} \qquad \text{(ii)} \quad t \geq \tau(R-1)$$

holds, then H_t *is the unique minimizer of* (LG_t) *in the class* $\mathscr{A}$*.*

The proof is based on a careful analysis of the competing terms in the energy. In both cases, a crucial step is to show that the radial-hedgehog is stable, i.e. the second variation is positive. In the case (i), the stability of the hedgehog is proved with the help of an Hardy-type inequality. In the case (ii), we adapt the methods of Ignat et al. [73], who prove the stability of the hedgehog in $\mathbb{R}^3$ for a different temperature regime. Once the stability is proved, we show that $|h_t| \simeq 1$ by applying the maximum principle. This information allows us to control the higher-order terms in the energy.

3 On Morse's index formula for VMO vector fields

In Chapter 4, which reports on a joint work with Segatti and Veneroni, we deal with a problem of a different nature. We consider a compact, orientable m-manifold with boundary $\mathscr{M} \subseteq \mathbb{R}^d$. We aim at characterizing the boundary data $\mathbf{g} \colon \partial\mathscr{M} \to \mathbb{S}^{d-1}$ such that there exists a $W^{1,m}$-unit vector field $\mathbf{v}$ satisfying $\mathbf{v} = \mathbf{g}$ on $\partial\mathscr{M}$. When $m = 2$, this problem is motivated by variational models of a thin liquid crystals film on a surface. In the simplest settings, the local orientation of the molecules is modeled by a unit vector field $\mathbf{v}$, and the energy functional has a quadratic growth in the gradient of $\mathbf{v}$. Therefore, it is natural to ask whether there exists $\mathbf{v}$ in the energy space subject to the assigned Dirichlet boundary conditions.

When $\mathbf{v}$, $\mathbf{g}$ are continuous, Morse's formula gives an answer by means of a topological invariant, namely, the index of a vector field. More precisely, Morse's formula reads

$$\mathrm{ind}(\mathbf{v}, \mathscr{M}) + \mathrm{ind}_-(\mathbf{v}, \partial\mathscr{M}) = \chi(\mathscr{M}). \tag{10}$$

The quantity $\mathrm{ind}(\mathbf{v}, \mathscr{M})$, called the *index* of the vector field, is an integer number depending on the behaviour of $\mathbf{v}$ around its zeros. The integer number $\mathrm{ind}_-(\mathbf{v}, \mathscr{M})$, which could be called the *inward boundary index*, depends on the behaviour of $\mathbf{v}$ on the portion of the boundary where $\mathbf{v}$ points inside $\mathscr{M}$. Both $\mathrm{ind}(\mathbf{v}, \mathscr{M})$ and $\mathrm{ind}_-(\mathbf{v}, \mathscr{M})$ are defined in terms of topological degree. Finally, $\chi(\mathscr{M})$ is the Euler-Poincaré characteristic of the manifold. Morse's formula implies that $\mathbf{g}$ can be extended to a continuous unit vector field if and only if

$$\mathrm{ind}_-(\mathbf{g}, \partial\mathscr{M}) = \chi(\mathscr{M}). \tag{11}$$

Since we aim at extending this characterization to vector fields of Sobolev regularity, we need to construct the index and the inward boundary index for non-continuous vector fields. We work in the Vanishing Mean Oscillation (VMO) class, which is the completion of $C^0(\mathscr{M})$ with respect to the Bounded Mean Oscillation (BMO) norm:

$$\|\mathbf{u}\|_{\mathrm{BMO}} := \sup_{\varepsilon>0,\ x\in\mathscr{M}} \fint_{B_\varepsilon^{\mathscr{M}}(x)} \left| \mathbf{u} - \fint_{B_\varepsilon^{\mathscr{M}}(x)} \mathbf{u} \,\mathrm{d}\mathscr{H}^m \right| \mathrm{d}\mathscr{H}^m.$$

This class contains the critical Sobolev spaces, that is

$$W^{s,p}(\mathscr{M}) \subseteq \mathrm{VMO}(\mathscr{M}) \qquad \text{when } sp = m,\ 1 \leq s < m.$$

In a sense, VMO functions are a good surrogate for continuous functions, because they support some topological constructions. In particular, a VMO degree theory has been developed by Brezis and Nirenberg in [25, 26]. Inspired by their work, and using essentially the density of continuous functions in VMO, we prove

Theorem 5 (C., Segatti and Veneroni, [31])**.** *Let $\mathscr{M} \subseteq \mathbb{R}^d$ be a compact, connected and orientable manifold with boundary. Assume that* $\mathbf{g} \in \mathrm{VMO}(\partial\mathscr{M}, \mathbb{R}^d)$ *satisfies*

$$\mathbf{g}(x) \in T_x\mathscr{M} \qquad \text{and} \qquad c_1 \leq |\mathbf{g}(x)| \leq c_2 \tag{12}$$

for some positive constants c_1, c_2 and a.e. $x \in \partial\mathscr{M}$. If $\mathbf{v} \in \mathrm{VMO}(\mathscr{M}, \mathbb{R}^d)$ has trace $\mathbf{g}$ (in the sense of Brezis and Nirenberg) and $\mathbf{v}(x) \in T_x\mathscr{M}$ for a.e. $x \in \mathscr{M}$, then (10) *holds. Moreover,* (11) *is a necessary and sufficient condition for the existence of a map $\mathbf{v} \in \mathrm{VMO}(\mathscr{M}, \mathbb{R}^d)$ with trace $\mathbf{g}$, such that*

$$\mathbf{v}(x) \in T_x\mathscr{M} \qquad \text{and} \qquad c_1 \leq |\mathbf{v}(x)| \leq c_2 \qquad \text{for a.e. } x \in \mathscr{M}.$$

If $\mathbf{g}$ satisfies $\mathbf{g} \in W^{1-1/p,p}(\mathscr{M}, \mathbb{R}^d)$ for $1 < p < +\infty$ in addition to (11)–(12), then $\mathbf{v}$ can be chosen in such a way that $\mathbf{v} \in W^{1,p}(\mathscr{M}, \mathbb{R}^d)$.

We also consider line fields on $\mathscr{M}$, i.e. assignments of an *unoriented* tangent direction to each point of $\mathscr{M}$. Line fields, compared to unit vector fields, are a more physically accurate way to describe nematic films on $\mathscr{M}$, because the nematic molecular director $\mathbf{n}$ possesses the reflection symmetry $\mathbf{n} \leftrightarrow -\mathbf{n}$. Using the formalism of Q-tensors, we define VMO line fields and prove a topological obstruction, namely a compact, orientable manifold $\mathscr{M}$ *without* boundary supports a VMO line field if and only if $\chi(\mathscr{M}) = 0$. It would be interesting to study line fields on a manifold with boundary. The main difficulty is topological in nature, as one needs to find an analogous of the index and Morse's formula for line fields with singularities. Combining a well-established geometrical theory with the methods of [31], it should be possible to establish topological constraints for singular line fields in VMO. However, we have not dealt with this problem yet, which could be the topic of a future work.

4 Perspectives and future work

In the analysis of minimizers of (LG$_\varepsilon$), several questions remain open. In particular, the picture in the three-dimensional case is far from being complete. A first question concerns the behaviour of the singular set $\mathscr{S}_{\mathrm{line}}$. We know that $\mathscr{S}_{\mathrm{line}}$ is 1-rectifiable and a stationary varifold. Unfortunately, this does not implies that $\mathscr{S}_{\mathrm{line}}$ is regular, in the classical sense. Indeed, the main regularity result for varifolds (i.e. Allard's theorem [3, Theorem 5.5]) assumes that the density Θ is integer-valued (or, more generally, it takes its values in a discrete set). Based on the Jerrard-Sandier type lower bound (5) and on (30), one could guess that

$$\Theta(x) = \kappa_* \qquad \text{for } \mathscr{H}^1\text{-a.e. } x \in \mathscr{S}_{\mathrm{line}}$$

(the $\geq$-inequality should follow from (5), whereas the $\leq$-inequality should be obtained by minimality). Then, Allard's theorem and the stationarity of $\mathscr{S}_{\mathrm{line}}$ would imply that $\mathscr{S}_{\mathrm{line}}$ is a union of line segments, connecting the point singularities of the boundary datum. At least in some simple cases, there should be no branching points (configurations without branching should be favorable in terms of length). So the question is: *is $\mathscr{S}_{\mathrm{line}}$ the union of non-intersecting straight lines?* Giving an answer based on comparison arguments alone seems quite delicate, as $\mathscr{S}_{\mathrm{line}}$ could have a rather complicated structure, with infinitely many components clustering around some point.

If additional information on the regularity of $\mathscr{S}_{\mathrm{line}}$ is known (in particular, if $\mathscr{S}_{\mathrm{line}}$ is a union of straight lines), then it would be interesting to study the structure of minimizers Q_ε in the core of line defects. For instance, *does the core of line defects contain biaxial phases?* In view of the results obtained in the two-dimensional case, one could expect that the answer is yes. A related issue is the analysis of *singularity profiles*. Let $x_0 \in \mathscr{S}_{\mathrm{line}}$ and let Π be an orthogonal plane to $\mathscr{S}_{\mathrm{line}}$, passing through the point x_0. Set

$$P_{\varepsilon,x_0}(y) := Q_\varepsilon(x_0 + \varepsilon y) \qquad \text{for } y \in \Pi.$$

This defines a bounded sequence in $L^\infty(\Pi, \mathbf{S}_0)$, such that

$$\|\nabla P_{\varepsilon,x_0}\|_{L^2(K)} = \|\nabla Q_\varepsilon\|_{L^2(x_0+\varepsilon K)} \leq C(K) \qquad \text{for every } K \subset\subset \Pi.$$

Therefore, up to a subsequence we have $P_{\varepsilon,x_0} \rightharpoonup P_{x_0}$ in $H^1_{\mathrm{loc}}(\Pi, \mathbf{S}_0)$. The map P_{x_0} contains the information on the fine structure of the defect core. What can be said about P_{x_0}? Is there a chance that P_{x_0} may actually be independent of x_0, at least in some very simple case (e.g., the boundary data are the same on every transversal slice)? How does the profile P_{x_0} relates to the solution of the two-dimensional problem?

By analogy with known results for the Ginzburg-Landau functional (see [2, 76]), one could conjecture that the Γ-*convergence*

$$I_\varepsilon := \frac{E_\varepsilon}{|\log \varepsilon|} \to I_0$$

holds. Here, the functional I_0 should be defined over a space of 1-currents, and it should account for the length of the topological line defects. The main issue is to understand the topology in which the Γ-convergence holds.

Finally, it could be interesting to study the behaviour of *more general functionals*. Indeed, the functional $(\mathrm{LG}_\varepsilon)$ is actually a simplified form of the full Landau-de Gennes energy:

$$\tilde{E}(Q) := \int_\Omega \left\{ L_1 \partial_k Q_{ij}\, \partial_j Q_{ik} + L_2 \partial_j Q_{ij}\, \partial_k Q_{ik} + L_3 \partial_k Q_{ij}\, \partial_k Q_{ij} + L_4 Q_{hl}\, \partial_h Q_{ij}\, \partial_l Q_{ij} + g(Q) \right\}.$$

When $L_4 \neq 0$ and $g = f$ is given by (3), the functional $\tilde{E}$ is unbounded from below (see [9, Proposition 4]). In this case, a more interesting choice of g is the singular potential proposed by Ball and Majumdar in [9]. With this choice of g, the functional remains bounded from below and minimizers exist even if $L_4 \neq 0$. A complete asymptotic analysis of $\tilde{E}$ with Ball-Majumdar's potential might be out of reach at the current state-of-the-art, and in any case it would require new ideas and techniques. However, one can hope to settle some simpler situations, e.g. the case $L_4 = 0$ and $g = f$. It would also be interesting to replace the quartic Landau-de Gennes' potential with another smooth potential, such as the sextic potential

$$f(Q) := -\frac{a_1}{2}\operatorname{tr} Q^2 - \frac{a_2}{3}\operatorname{tr} Q^3 + \frac{a_3}{4}\left(\operatorname{tr} Q^2\right)^2 + \frac{a_4}{5}\left(\operatorname{tr} Q^2\right)\left(\operatorname{tr} Q^3\right) + \frac{a_5}{6}\left(\operatorname{tr} Q^2\right)^3 + \frac{a_5'}{6}\left(\operatorname{tr} Q^3\right)^2$$

(see [36, 58]). In this case, the topological structure of the problem may change dramatically, for instance the vacuum manifold may contain biaxial tensors.

The thesis is organized as follows. In Chapter 1, we discuss the problem in a two-dimensional domain, and we prove the results stated in Subsection 0.2.1. In Chapter 2, we present the asymptotic analysis in a three-dimensional domain. The analysis of the low temperature limit on a spherical shell is contained in Chapter 3. Finally, Chapter 4 is devoted to Morse's index formula for VMO vector fields.

Biaxialité et analyse asymptotique pour le modèle de Landau-de Gennes en dimension deux

Dans ce travail, nous étudions le modèle variationnel de Landau-de Gennes dans un domaine borné et régulier en dimension 2. Nous montrons que le minimiseurs sont très fortement biaxes au voisinages des défauts, c'est-à-dire, le paramètre de biaxialité atteint la valeur 1 qui est la valeur maximale possible. Ensuite, nous nous intéressons à l'analyse asymptotique des minimiseurs lorsque la constante élastique tend vers zéro. L'étude asymptotique est mis en place dans un cadre plus général, qui permet de récupérer la fonctionnelle de Landau-de Gennes en tant que cas particulier.

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Chapter 1

Biaxiality in the asymptotic analysis of a two-dimensional Landau-de Gennes model

Abstract

We consider the Landau-de Gennes variational problem on a bounded, two dimensional domain, subject to Dirichlet smooth boundary conditions. We prove that minimizers are maximally biaxial near the singularities, that is, their biaxiality parameter reaches the maximum value 1. Moreover, we discuss the convergence of minimizers in the vanishing elastic constant limit. Our asymptotic analysis is performed in a general setting, which recovers the Landau-de Gennes problem as a specific case.

Contents

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1.1 Introduction

Nematic liquid crystals are an intermediate phase of matter, which shares some properties both with solid and liquid states. They are composed by rigid, rod-shaped molecules which can flow freely, as in a conventional liquid, but tend to align locally along some directions, thus recovering, to some extent, long-range orientational order. As a result, liquid crystals behave mostly like fluids, but exhibit anisotropies with respect to some optical or electromagnetic properties, which makes them suitable for many applications.

In the mathematical and physical literature about liquid crystals, different continuum theories have been proposed. Some of them — like the Oseen-Frank and the Ericksen theories — postulate that, at every point, the molecules tend to align along a preferred direction, so that the resulting configuration has an axis of rotational symmetry. Such a behaviour is commonly referred to as *uniaxiality.* In contrast, the Landau-de Gennes theory, which is considered here, allows *biaxiality.* In a biaxial arrangement, there is no axis of rotational symmetry, but there are three orthogonal axes of reflection symmetry. There is experimental evidence for biaxiality in thermotropic materials, that is, materials whose phase transitions are induced by temperature (see [1, 94]).

In the Landau-de Gennes theory (or, as it is sometimes informally called, the Q-tensor theory), the local configuration of the liquid crystal is modeled with a real 3×3 symmetric traceless matrix $Q(x)$, depending on the position x. The set of Q-tensors can be defined as

$$\mathbf{S}_0 := \left\{ Q \in \mathrm{M}_3(\mathbb{R}) \colon Q^{\mathsf{T}} = Q, \ \operatorname{tr} Q = 0 \right\}.$$

This is a real linear space, of dimension five, which we endow with the scalar product $Q \cdot P := Q_{ij} P_{ij}$ (Einstein's convention is assumed). The configurations are classified according to the eigenvalues of Q. *Isotropic* (i.e., totally lacking of symmetry) states correspond to $Q = 0$. Matrices $Q \neq 0$ with two equal eigenvalues describe *uniaxial* configurations, which have an axis of rotational symmetry. Finally, matrices Q with distinct eigenvalues represents *biaxial* configurations, which have three orthogonal axes of reflection symmetry but no rotational symmetry. The biaxiality of a matrix $Q \in \mathbf{S}_0 \setminus \{0\}$ is measured by the parameter

$$\beta(Q) := 1 - 6 \frac{\left(\operatorname{tr} Q^3\right)^2}{\left(\operatorname{tr} Q^2\right)^3},$$

ranging in $[0, 1]$, such that $\beta(Q) = 0$ if and only if Q is uniaxial. Every Q-tensor can be represented as follows:

$$Q = s \left\{ \left(\mathbf{n}^{\otimes 2} - \frac{1}{3} \operatorname{Id} \right) + r \left(\mathbf{m}^{\otimes 2} - \frac{1}{3} \operatorname{Id} \right) \right\} \tag{1.1.1}$$

with $0 \leq r \leq 1$, $s \geq 0$ and $(\mathbf{n}, \mathbf{m})$ is a positively oriented orthonormal pair in $\mathbb{R}^3$. The number s is the scalar order parameter, which measures the degree of order of the configuration, whereas r is related to biaxiality. (in particular, the biaxiality parameter $\beta(Q)$ can be written as a function of r). The vectors $\mathbf{n}$ and $\mathbf{m}$ describe the orientation of the symmetry axes. A matrix is uniaxial if and only if $s > 0$ and $r \in \{0, 1\}$. In the uniaxial case, the director of the rotational symmetry axis is either $\mathbf{n}$ (when $r = 0$) or $\mathbf{n} \times \mathbf{m}$ (when $r = 1$), whereas in the biaxial case the axes of reflection symmetry are identified by $(\mathbf{n}, \mathbf{m}, \mathbf{n} \times \mathbf{m})$. Here, $\times$ denotes the vector product in $\mathbb{R}^3$. The geometry of the space of Q-tensors is represented in Figure 1.1.

In this chapter, we consider first a two-dimensional model. The material is contained in a bounded, smooth domain $\Omega \subseteq \mathbb{R}^2$, subject to smooth Dirichlet boundary conditions. We consider the Landau-de Gennes energy functional in its simplest form,

$$E_\varepsilon(Q) = \int_\Omega \left\{ \frac{1}{2} \left| \nabla Q \right|^2 + \frac{1}{\varepsilon^2} f(Q) \right\}. \tag{LG$_\varepsilon$}$$

Here f is the bulk potential, given by

$$f(Q) = k_0 - a \operatorname{tr} Q^2 - b \operatorname{tr} Q^3 + c \left(\operatorname{tr} Q^2 \right)^2. \tag{1.1.2}$$

The positive parameters a, b and c depend on the material and the temperature. The constant k_0 is chosen in such a way that $\inf f = 0$. It can be proved (see [9, Proposition 9]) that f attains its minimum

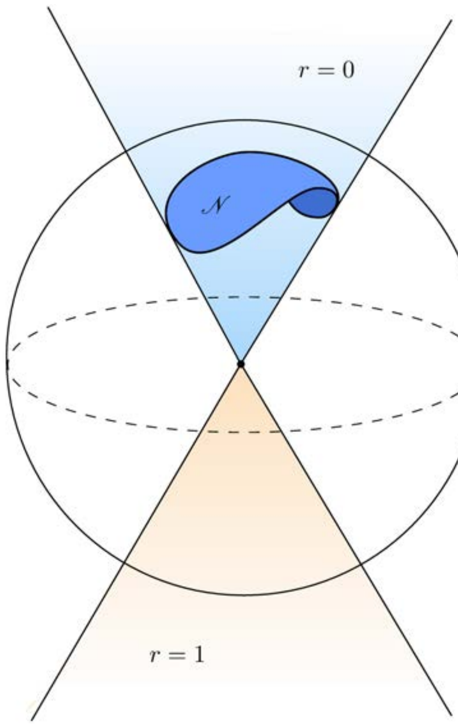

Figure 1.1: The space of Q-tensors. The unit sphere and the uniaxial cones, corresponding to $r = 0$ and $r = 1$, are represented. The vacuum manifold is the intersection between the sphere and the cone $r = 0$.

on a manifold $\mathscr{N}$, called the vacuum manifold, whose elements are the matrices which have $s = s_*$, $r = 0$ in the representation formula (1.1.1) for some $s_* = s_*(a, b, c) > 0$. The potential energy $\varepsilon^{-2} f(Q)$ penalizes the constraint $Q \in \mathscr{N}$. The parameter ε^2 is a material-dependent elastic constant, which is typically very small (of the order of 10^{-11} Jm^{-1}): this motivates our interest in the limit as $\varepsilon \searrow 0$.

Due to the form of the functional (LG$_\varepsilon$), there are some similarities between this problem and the Ginzburg-Landau model for superconductivity, where the configuration space is the complex field $\mathbb{C} \simeq \mathbb{R}^2$, the energy is given by

$$E_\varepsilon(u) = \int_\Omega \left\{ \frac{1}{2} |\nabla u|^2 + \frac{1}{4\varepsilon^2} \left(1 - |u|^2\right)^2 \right\}$$

and the vacuum manifold is the unit circle. The convergence analysis for this model is a widely addressed issue in the literature (see, for instance, [14] for the study of the 2D case). A well-known phenomenon is the appearance of the so-called topological defects. Depending on the homotopic properties of the boundary datum, there might be an obstruction to the existence of smooth maps $\Omega \to \mathscr{N}$. Boundary data for which this obstruction occurs will be referred to as homotopically non-trivial (see Subsection 1.2.1). In this case, the image of minimizers fails to lie close to the vacuum manifold on some small set which correspond, in the limit as $\varepsilon \searrow 0$, to the singularities of the limit map.

In the Ginzburg-Landau model, the whole configuration space $\mathbb{C}$ can be recovered as a topological cone over the vacuum manifold. In other words, every configuration $u \in \mathbb{C} \setminus \{0\}$ is identified by its modulus and phase, the latter being associated with an element of the vacuum manifold. Defects are characterized as the regions where $|u|$ is small. This structure is found in other models: for instance, let us mention the contribution of Chiron [33], who replaced $\mathbb{C}$ by a cone over a generic compact, connected manifold.

In contrast, in the Landau-de Gennes model the target space *cannot* be identified as a cone over the vacuum manifold. Since $\mathscr{N}$ has codimension 3 in $\mathbf{S}_0$, several behaviours are possible for minimizers, in the core of the defects. For instance, one might ask whether the minimizing configurations contain isotropic and/or biaxial points. From this point of view, a relevant parameter to consider is the temperature, which is involved in the problem through the potential f. Indeed, letting T_0 be the temperature at which the isotropic-nematic phase transition occurs, and $T < T_0$ the temperature of the sample, we have

$$t := \frac{ac}{b^2} \propto T_0 - T.$$

Large values of t correspond to low temperatures.

Numerical simulations suggest that we might expect biaxiality in the core of defects. In particular, Schopohl and Sluckin (see [128]) claimed that the core is heavily biaxial, and that it does not contain isotropic liquid. Gartland and Mkaddem [51] proved that, when Ω is a ball in $\mathbb{R}^3$ and the radius is large enough, the unique uniaxial, radially symmetric critical point of (P_ε) — called radial-hedgehog — is unstable for $t \gg 1$. Ignat et al. [73] proved the instability of the radial-hedgehog on the whole space $\mathbb{R}^3$, when $t \gg 1$. (They also showed that the radial-hedgehog is stable when $t \ll 1$.) Henao and Majumdar [71] proved that the minimizers cannot be purely uniaxial, when t is large enough. Later on, Lamy [83] showed that actually, the radial-hedgehog is the unique purely uniaxial critical point of the Landau-de Gennes' energy. In particular, Henao and Majumdar's theorem is a corollary of Gartland and Mkaddem's result. Lamy also proved that, in a two-dimensional domain, every uniaxial critical point can be written as

$$Q(x) = s(x) \left(\mathbf{n}_0^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right)$$

for a constant $\mathbf{n}_0$. Therefore, purely uniaxial critical points cannot exist if the boundary data is non-trivial. Finally, a special biaxial configuration, known as "biaxial torus", has been identified in the core of point defects of degree 1, in three-dimensional domains (see [51, 81, 82, 132]).

However, these results do not exclude that minimizers are "almost uniaxial", i. e., their degree of biaxiality is small everywhere, so that they do not differ significantly from a pure uniaxial state. The results we prove in this chapter rule out this possibility. Our first result deals with minimizers in a two-dimensional domain, in the low temperature regime.

Theorem 1.1.1. *Assume that the boundary datum $g \in C^1(\partial\Omega, \mathscr{N})$ is homotopically non-trivial (see Definition 1.2.1). There exist positive numbers $t_0 = t_0(\Omega, g)$ and $\varepsilon_0 = \varepsilon_0(\Omega, g, a, b, c)$ such that, if the conditions*

$$\frac{ac}{b^2} \geq t_0 \qquad \text{and} \qquad \varepsilon \leq \varepsilon_0$$

hold, then any minimizer Q_ε of $(\mathrm{LG}_\varepsilon)$ satisfies

$$\min_{\overline{\Omega}} |Q_\varepsilon| > 0 \qquad \text{and} \qquad \max_{\overline{\Omega}} \beta(Q_\varepsilon) = 1.$$

Theorem 1.1.1 prevents the isotropic phases ($Q = 0$) from appearing in minimizers, in the low temperature regime. This is a remarkable difference between the Landau-de Gennes theory and the popular Ericksen model for liquid crystals: in the latter, defects are always associated with isotropic melting, since biaxiality is not taken into account. Remark that Theorem 1.1.1 is in agreement with the conclusions of [128].

The proof of this result relies on energy estimates. With the help of the coarea formula, we are able to bound from below the energy of any uniaxial configuration. Then, we provide an explicit example of maximally biaxial solution, whose energy is smaller than the bound we have obtained, and we conclude that uniaxial minimizers cannot exist.

Another topic we discuss in this chapter is the convergence of minimizers as $\varepsilon \searrow 0$. It turns out that a convergence result for the minimizers of $(\mathrm{LG}_\varepsilon)$ can be established without any need to exploit the matricial structure of the configuration space, nor the precise shape of f and $\mathscr{N}$. For this reason, we will be interested in the asymptotic analysis of a more general functional:

$$E_\varepsilon(u) := \int_\Omega \left\{ \frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} f(u) \right\},$$

Here the function u takes values in an Euclidean space $\mathbb{R}^d$, and $f\colon \mathbb{R}^d \to \mathbb{R}$ is a smooth, non-negative function, such that $\mathscr{N} := f^{-1}(0)$ is a smooth, compact and connected manifold. We impose Dirichlet boundary condition $u_{|\partial\Omega} = g$, where $g \in C^1(\partial\Omega, \mathscr{N})$. The potential f and the datum g are assumed to satisfy the conditions (H$_1$)–(H$_5$), listed in Section 1.2. We denote by u_ε any minimizer of the general functional.

Proposition 1.1.2. *Assume that conditions (H$_1$)–(H$_5$) hold. There exist some ε-independent constants λ_0, $\delta_0 > 0$ and, for each $\delta \in (0, \delta_0)$, a finite set $X_\varepsilon = X_\varepsilon(\delta) \subseteq \Omega$, whose cardinality is bounded independently of ε, such that*

$$\operatorname{dist}(x, X_\varepsilon) \geq \lambda_0 \varepsilon \qquad \textit{implies that} \qquad \operatorname{dist}(u_\varepsilon(x), \mathscr{N}) \leq \delta.$$

The set X_ε is empty if and only if the boundary datum is homotopically trivial. In the Landau-de Gennes case (LG$_\varepsilon$)–(1.1.2), Proposition 1.1.2 and Theorem 1.1.1, combined, show that a minimizer Q_ε is "almost uniaxial" everywhere, except on k balls of radius comparable to ε, where biaxiality occurs. Actually, we will prove that $k = 1$ (see Proposition 1.1.4).

We can show that the minimizers converge, as $\varepsilon \searrow 0$, to a map taking values in $\mathscr{N}$, having a finite number of singularities. Moreover, due to the variational structure of the problem, the limit map is optimal, in some sense, with respect to the Dirichlet integral $v \mapsto \frac{1}{2}\int_\Omega |\nabla v|^2$.

Theorem 1.1.3. *Under the assumptions (H$_1$)–(H$_5$), there exists a subsequence $\varepsilon_n \searrow 0$, a finite set $X \subseteq \Omega$ and a function $u_0 \in C^\infty(\Omega \setminus X, \mathscr{N})$ such that*

$$u_{\varepsilon_n} \to u_0 \qquad \textit{strongly in } H^1_{\mathrm{loc}} \cap C^0(\Omega \setminus X, \mathbb{R}^d).$$

On every ball $B \subset\subset \Omega \setminus X$, the function u_0 is minimizing harmonic, which means

$$\frac{1}{2}\int_B |\nabla u_0|^2 = \min\left\{ \frac{1}{2}\int_B |\nabla v|^2 : v \in H^1(B, \mathscr{N}),\ v = u_0 \textit{ on } \partial B \right\}.$$

In particular, u_0 is a solution of the harmonic map equation

$$\Delta u_0(x) \perp T_{u_0(x)}\mathscr{N} \qquad \text{for all } x \in \Omega \setminus X,$$

where $T_{u_0(x)}\mathscr{N}$ is the tangent plane of $\mathscr{N}$ at the point $u_0(x)$ and the symbol $\perp$ denotes orthogonality.

We can provide some information about the behaviour of u_0 around the singularity. For the sake of simplicity, we assume here that $\mathscr{N}$ is the real projective plane $\mathbb{RP}^2$ (this is the case, for instance, of the Landau-de Gennes potential (1.1.2)).

Proposition 1.1.4. *In addition to (H$_1$)–(H$_4$), assume that $\mathscr{N} \simeq \mathbb{RP}^2$ and the boundary datum is non-trivial (see Definition 1.2.1). Then, X reduces to a singleton $\{a\}$. For $\rho \in (0, \operatorname{dist}(a, \partial\Omega))$, consider the function $\mathbb{S}^1 \to \mathscr{N}$ given by*

$$c_\rho\colon \theta \mapsto u_0\left(a + \rho e^{i\theta}\right).$$

Up to a subsequence $\rho_n \searrow 0$, $\{c_{\rho_n}\}_{n\in\mathbb{N}}$ converges uniformly (and in $C^{0,\alpha}$ for $\alpha < 1/2$) to a geodesic c_0 in $\mathscr{N}$, which minimizes the length among the homotopically non-trivial loops in $\mathscr{N}$.

Unfortunately, we have not been able to prove the convergence for the whole family $\{c_\rho\}_{\rho>0}$, which remains still an open question.

An interesting question, related to the topics we discuss in this chapter, is the study of the singularity profile for defects in the Landau-de Gennes model. Consider a singular point $a \in X$, and set $P_\varepsilon(x) := Q_\varepsilon(a + \varepsilon x)$ for all $x \in \mathbb{R}^2$ for which this expression is well-defined. Then P_ε is a bounded family in L^∞ (see Lemma 1.4.1) and it is clear, by scaling arguments, that

$$\|\nabla P_\varepsilon\|_{L^2(K)} \leq C \qquad \text{for all } K \subset\subset \mathbb{R}^2.$$

Thus, up to a subsequence, $\{P_\varepsilon\}$ converges weakly in $H^1_{\mathrm{loc}}(\mathbb{R}^2)$ to some P_*. It is readily seen that, for each $R > 0$, P_* minimizes in $B(0, R)$ the functional E_1 among the functions $P \in H^1(B(0, R))$ satisfying $P = P_*$ on $\partial B(0, R)$, and consequently it solves in $\mathbb{R}^2$ the Euler-Lagrange equation associated with E_1. A function P_* obtained by this construction is called a singularity profile. Understanding the properties of such a profile will lead to a deeper comprehension of what happens in the core of defects, and vice-versa. Remark that, in view of Theorem 1.1.1, strong biaxiality has to be found in singularity profiles corresponding to low temperatures. Profiles of point defects in the two-dimensional Landau-de Gennes model have been studied in detail by Di Fratta et al., in a recent paper [41]. For the three-dimensional case, let us mention the paper by Henao and Majumdar [71], where a spherical droplet, with radially symmetric boundary conditions, is considered. Restricting the problem to the class of uniaxial Q-tensors, the authors proved convergence to a radial-hedgehog profile. (Actually, Lamy has recently claimed a stronger result, namely, the radial hedgehog is the only uniaxial critical point for the Landau-de Gennes energy — see [83, Theorem 5.1]).

This chapter is organized as follows. In Section 1.2 we present in detail our general problem, we set notations, and we introduce some tools for the subsequent analysis. More precisely, in Subsection 1.2.1 we define the energy cost of a defect, and in Subsection 1.2.2 we discuss the nearest point projection on a manifold. Section 1.3 specifically pertains to the Q-tensor model, and contains the proof of Theorem 1.1.1. The asymptotic analysis, with the proof of Proposition 1.1.2 and Theorem 1.1.3, is provided in Section 1.4. Finally, Section 1.5 deals with Proposition 1.1.4.

1.2 Setting of the general problem and preliminaries

As we mentioned in the introduction, our asymptotic analysis will be carried out in a general setting, which recovers the Landau-de Gennes model (LG_ε)–(1.1.2) as a particular case. In this section, we detail the problem under consideration. The unknown is a function $\Omega \to \mathbb{R}^d$, where Ω is a smooth, bounded (and possibly not simply connected) domain in $\mathbb{R}^2$. Let $g \colon \partial\Omega \to \mathbb{R}^d$ be a boundary datum, and define the Sobolev space $H^1_g(\Omega, \mathbb{R}^d)$ as the set of maps in $H^1(\Omega, \mathbb{R}^d)$ which agrees with g on the boundary, in the sense of traces. We are interested in the problem

$$(\mathrm{P}_\varepsilon) \qquad \min_{u \in H^1_g(\Omega, \mathbb{R}^d)} E_\varepsilon(u)$$

where

$$E_\varepsilon(u) := E_\varepsilon(u, \Omega) = \int_\Omega \left\{ \frac{1}{2} |\nabla u|^2 + \frac{1}{\varepsilon^2} f(u) \right\}$$

and $f \colon \mathbb{R}^d \to \mathbb{R}$ is a non negative, smooth function, satisfying the assumptions below. The existence of a minimizer for Problem (P_ε) can be easily inferred via the Direct Method in the calculus of variations. If u_ε denotes a minimizer for E_ε, then u_ε is a weak solution of the Euler-Lagrange equation

$$(1.2.1) \qquad -\Delta u_\varepsilon + \frac{1}{\varepsilon^2} \mathrm{D} f(u_\varepsilon) = 0 \qquad \text{in } \Omega.$$

Via elliptic regularity theory, it can be proved that every solution of (1.2.1) is smooth.

Assumptions on the potential and on the boundary datum. Denote, as usual, by $\mathbb{S}^{d-1}$ the unit sphere of R^d, and by $\mathrm{dist}(v, N)$ the distance between a point $v \in \mathbb{R}^d$ and a set N. We assume that $f \colon \mathbb{R}^d \to \mathbb{R}$ is a smooth function (at least of class $C^{2,1}$), satisfying the following conditions:

(H_1) We have $f \geq 0$, the set $\mathscr{N} := f^{-1}(0)$ is non-empty, and $\mathscr{N}$ is a smooth, compact and connected submanifold of $\mathbb{R}^d$, without boundary.

(H_2) There exist some positive constants $\delta_0 < 1$, m_0 such that, for all $v \in \mathscr{N}$ and all normal vector $\nu \in \mathbb{R}^d$ to $\mathscr{N}$ at the point v,

$$\mathrm{D}f(v + t\nu) \cdot \nu \geq m_0 t, \qquad \text{if } 0 \leq t \leq \delta_0.$$

(H_3) For all $v \in \mathbb{R}^d$ with $|v| > 1$, we have

$$f(v) > f\left(\frac{R_0 v}{|v|}\right),$$

where R_0 is a positive constant such that $\mathscr{N}$ is contained in the closed ball of radius R_0.

The set $\mathscr{N}$ will be referred as the vacuum manifold. Up to rescaling the norm in $\mathbb{R}^d$, throughout our analysis we assume that $R_0 = 1$. As for the boundary datum, we assume

(H_4) $g\colon \partial\Omega \to \mathbb{R}^d$ is a smooth function, and $g(x) \in \mathscr{N}$ for all $x \in \partial\Omega$.

For technical reasons, we impose a restriction on the homotopic structure of $\mathscr{N}$. A word of clarification: by conjugacy class in a group G, we mean any set of the form $\{axa^{-1}\colon a \in G\}$, for $x \in G$.

(H_5) Every conjugacy class in the fundamental group of $\mathscr{N}$ is finite.

Remark 1.2.1. The assumption (H_2) holds true if, at every point $v \in \mathscr{N}$, the Hessian matrix $\mathrm{D}^2 f(v)$ restricted to the normal space of $\mathscr{N}$ at v is positive definite. Hence, (H_2) may be interpreted as a *non-degeneracy* condition for f, in the normal directions.

Remark 1.2.2. We can provide a sufficient condition for (H_3) as well, namely

$$v \cdot \mathrm{D}f(v) > 0 \qquad \text{for } |v| > R_0$$

(for this implies $\mathrm{d}f(tv)/\mathrm{d}t > 0$ for $t > R_0$). Hypothesis (H_3) is exploited uniquely in the proof of the L^∞-bound for u_ε.

Remark 1.2.3. Assumption (H_5) is trivially satisfied if the fundamental group $\pi_1(\mathscr{N})$ is abelian or finite. This covers many cases, arising from other models in condensed matter physic. Besides rod-shaped molecules in nematic phase, we mention planar spins ($\mathscr{N} \simeq \mathbb{S}^1$) and ordinary spins ($\mathscr{N} \simeq \mathbb{S}^2$), biaxial molecules in nematic phase ($\mathscr{N} \simeq SU(2)/H$, where H is the quaternion group), super-fluid He-3, both in dipole-free and dipole-locked phases ($\mathscr{N} \simeq (SU(2) \times SU(2))/H$ and $\mathscr{N} \simeq \mathbb{RP}^3$, respectively).

The Landau-de Gennes model. In this model, the configuration parameter belongs to the set $\mathbf{S}_0$ of matrices, given by

$$\mathbf{S}_0 := \left\{Q \in \colon Q^\mathsf{T} = Q, \ \operatorname{tr} Q = 0\right\}.$$

This is a real linear space, whose dimension, due to the symmetry and tracelessness constraints, is readily seen to be five. The tensor contraction $Q \cdot P = \operatorname{tr}(QP) = \sum_{i,j} Q_{ij} P_{ij}$ defines a scalar product on $\mathbf{S}_0$, and the corresponding norm will be denoted $|\cdot|$. Clearly $\mathbf{S}_0$ can be identified, up to an equivalent norm, with the Euclidean space $\mathbb{R}^5$. In this model, the potential is given by

$$f(Q) := k_0 - \frac{a}{2} \operatorname{tr} Q^2 - \frac{b}{3} \operatorname{tr} Q^3 + \frac{c}{4} \left(\operatorname{tr} Q^2\right)^2 \qquad \text{for all } Q \in \mathbf{S}_0, \tag{1.2.2}$$

where a, b, c are positive parameters and k_0 is a properly chosen constant, such that $\inf f = 0$. It is clear that the minimization problem does not depend on the value of k_0. (We have set $a := -\alpha(T - T_*)$ in formula (1.1.2).) In the Euler-Lagrange equation for this model, $\mathrm{D}f$ has to be intended as the intrinsic gradient with respect to $\mathbf{S}_0$. Since the latter is a proper subspace of the 3×3 real matrices, $\mathrm{D}f$ contains an extra term, which acts as a Lagrange multiplier associated with the tracelessness constraint. Therefore, denoting by Q_ε any minimizer, Equation (1.2.1) reads

$$-\varepsilon^2 \Delta Q_\varepsilon - aQ_\varepsilon - b\left\{Q_\varepsilon^2 - \frac{1}{3}(\operatorname{tr} Q_\varepsilon^2)\,\mathrm{Id}\right\} + cQ_\varepsilon \operatorname{tr} Q_\varepsilon^2 = 0, \tag{1.2.3}$$

where the term proportional to Id is the Lagrange multiplier. As we show in Subsection 1.3.1, (1.2.2) fulfills the conditions (H_1)–(H_5), thus it can be recovered in the general setting.

1.2.1 Energy cost of a defect

By the theory of continuous media, it is well known (see [99]) that topological defects of codimension two are associated with homotopy classes of loops in the vacuum manifold $\mathscr{N}$. Now, following an idea of [33], we are going to associate to each homotopy class a non negative number, representing the energy cost of the defect. Let $\Gamma(\mathscr{N})$ be the set of free homotopy classes of loops $\mathbb{S}^1 \to \mathscr{N}$, that is the set of the path-connected components of $C^0(\mathbb{S}^1, \mathscr{N})$ — here, "free" means that no condition on the base point is imposed. As is well-known, for a fixed base point $v_0 \in \mathscr{N}$ there exists a one-to-one and onto correspondence between $\Gamma(\mathscr{N})$ and the conjugacy classes of the fundamental group $\pi_1(\mathscr{N}, v_0)$. As the latter might not be abelian, the set $\Gamma(\mathscr{N})$ is not a group, in general. Nevertheless, the composition of paths (denoted by $*$) induces a map

$$\Gamma(\mathscr{N}) \times \Gamma(\mathscr{N}) \to \mathscr{P}\left(\Gamma(\mathscr{N})\right), \qquad (\alpha, \beta) \mapsto \alpha \cdot \beta \tag{1.2.4}$$

in the following way: for each $v \in \mathscr{N}$, fix a path c_v connecting v_0 to v. Then, for $\alpha, \beta \in \Gamma(\mathscr{N})$ define

$$\alpha \cdot \beta := \left\{\text{homotopy class of the loop } ((c_{f(1)} * f) * \widetilde{c_{f(1)}}) * ((c_{g(1)} * g) * \widetilde{c_{g(1)}})\colon f \in \alpha,\, g \in \beta\right\},$$

where $\widetilde{c_{f(1)}}$, $\widetilde{c_{g(1)}}$ are the reverse paths of $c_{f(1)}$, $c_{g(1)}$ respectively. If we regard α, β as conjugacy classes in $\pi_1(\mathscr{N}, v_0)$, we might check that

$$\alpha \cdot \beta = \{\text{conjugacy class of } ab\colon a \in \alpha,\, b \in \beta\}$$

(in particular, we see that $\alpha \cdot \beta$ does not depend on the choice of $(c_v)_{v \in \mathscr{N}}$). As α, β are finite, due to (H_5), the set $\alpha * \beta$ is finite as well.

The set $\Gamma(\mathscr{N})$, equipped with this product, enjoys some algebraic properties, which descend from the group structure of $\pi_1(\mathscr{N}, v_0)$. The resulting structure is referred to as the polygroup of conjugacy classes of $\pi_1(\mathscr{N}, v_0)$, and was first recognized by Campaigne (see [28]) and Dietzman (see [42]). We remark that, even if $\pi_1(\mathscr{N}, b)$ is not abelian, we have $\alpha \cdot \beta = \beta \cdot \alpha$ for all $\alpha, \beta \in \Gamma(\mathscr{N})$. This follows from $ab = a(ba)a^{-1}$, which holds true for all $a, b \in \pi_1(\mathscr{N}, v_0)$.

The geometric meaning of the map (1.2.4) is captured by the following proposition. By convention, let us set $\prod_{i=1}^1 \gamma_i := \{\gamma_1\}$.

Lemma 1.2.1. *Let D be a smooth, bounded domain in $\mathbb{R}^2$, whose boundary has $k \geq 2$ connected components, labeled $C_1, \ldots, C_k$. For all $i = 1, \ldots, k$, let $g_i\colon C_i \to \mathscr{N}$ be a smooth boundary datum, whose free homotopy class is denoted by γ_i. If the condition*

$$\prod_{i=1}^{h} \gamma_i \cap \prod_{i=h+1}^{k} \gamma_i \neq \emptyset \tag{1.2.5}$$

holds for some index h, then there exists a smooth function $g\colon \overline{D} \to \mathscr{N}$, which agrees with g_i on every C_i. Conversely, if such an extension exists then the condition (1.2.5) holds for all $h \in \{1, \ldots, k\}$.

Proof. Throughout the proof, given a path c we will denote the reverse path by $\tilde{c}$.

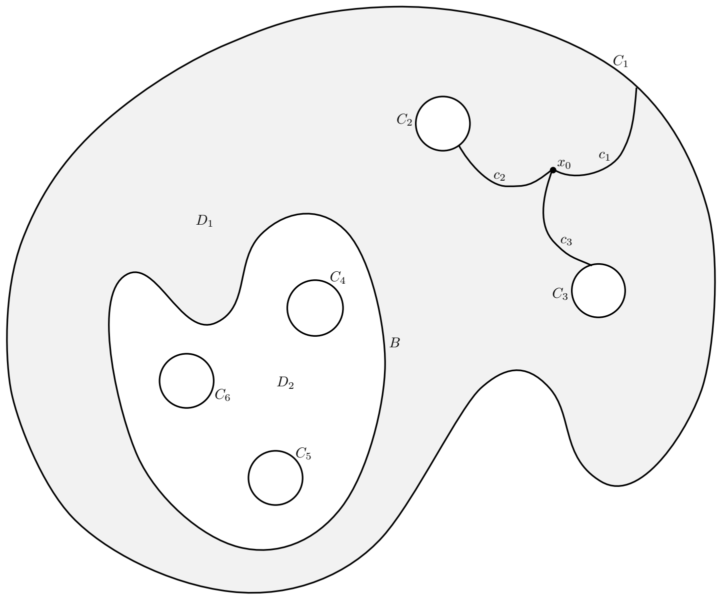

Figure 1.2: The geometry of D' in Lemma 1.2.1.

Assume that (1.2.5) holds. We claim that the boundary data can be extended continuously on D. It is convenient to work out the construction in the subdomain

$$D' := \{x \in D \colon \operatorname{dist}(x, D) > \delta\},$$

where $\delta > 0$ is small, so that D and D' have the same homotopy type. Up to a diffeomorphism, we can suppose that D' is a disk with k holes, and C_1 is the exterior boundary. It is equally fair to assume that there exists a path B, homeomorphic to a circle, which splits D' into two regions, D_1 and D_2, with

$$\partial D_1 = B \cup \bigcup_{i=1}^{h} C_i, \qquad \partial D_2 = B \cup \bigcup_{i=h+1}^{k} C_i.$$

This configuration is illustrated in Figure 1.2. Let $b \colon B \to \mathscr{N}$ be a loop whose free homotopy class belongs to $\prod_{i=1}^{h} \gamma_i \cap \prod_{i=h+1}^{k} \gamma_i$.

We wish, at first, to extend the boundary data to a continuous function defined on D_1. Let $c_1, \ldots, c_h$ be mutually non intersecting paths $[0, 1] \to D_1$, connecting a fixed base point $x_0 \in D_1$ with $C_1, \ldots, C_h$ respectively, and let Σ denote the union of $C_1, \ldots, C_h$ and the images of $c_1, \ldots, c_h$. The set Σ can be parametrized by the loop

$$\alpha := ((c_1 * \alpha_1) * \widetilde{c_1}) * ((c_2 * \alpha_2) * \widetilde{c_2}) * \cdots * ((c_h * \alpha_h) * \widetilde{c_h}),$$

where $\alpha_i \colon [0, 1] \to C_i$ is a parametrization of C_i proportional to arc length.

Next, we "push forward" α to a loop in $\mathscr{N}$. Since $b \in \prod_{i=1}^{h} \gamma_i$, there exists a loop σ, freely homotopic to b, which can be written as

$$\sigma := ((\sigma_1 * g_1') * \tilde{\sigma}_1) * ((\sigma_2 * g_2') * \tilde{\sigma}_2) * \cdots * ((\sigma_h * g_h') * \tilde{\sigma}_h),$$

where $g_i' \in \gamma_i$ and σ_i is a path in $\mathscr{N}$ connecting a fixed base point $v_0 \in \mathscr{N}$ with $g_i'(1)$, for each $i \in \{1, 2, \ldots, h\}$. We can regard σ as a map $\Sigma \to \mathscr{N}$: more precisely, we can set $t \in [0, 1] \mapsto \sigma(\alpha^{-1}(t))$

and check that this mapping is well-defined. By construction, there exists a homotopy between b and σ, which provides a continuous extension of the boundary data $g'_1, \ldots, g'_h$, b to a mapping $v_1\colon D_1 \to \mathscr{N}$.

We perform the same construction on the subdomain D_2, obtaining a continuous function v_2. Pasting v_1 and v_2 we get a continuous map $v'\colon \overline{D}' \to \mathscr{N}$, whose trace on each C_i is homotopic to g_i. As $D \setminus D'$ is just a small neighborhood of ∂D, it is not difficult to extend v' to a continuous function $v\colon \overline{D} \to \mathscr{N}$, such that $v_{|C_i} = g_i$ for all i. Smoothness can be recovered, for instance, via a standard approximation argument.

Conversely, assume that an extension g exists, and let B, D_1, D_2, Σ be as before, for h arbitrary. Then, $g_{|D_1}$ provides a free homotopy between $g_{|B}$ and $g_{|\Sigma}$, so the homotopy class of $g_{|B}$ belongs to $\prod_{i=1}^h \gamma_i$. Similarly, the class of $g_{|B}$ belongs to $\prod_{i=h+1}^k \gamma_i$, and hence the condition 1.2.5 holds. □

For each $\gamma \in \Gamma(\mathscr{N})$, we define its length as

$$\lambda(\gamma) := \inf\left\{\left(2\pi\int_{\mathbb{S}^1} |c'(\theta)|^2 \, \mathrm{d}\theta\right)^{1/2} : c \in \gamma \cap H^1(\mathbb{S}^1, \mathscr{N})\right\}. \tag{1.2.6}$$

First, the set $\gamma \cap H^1(\mathbb{S}^1, \mathscr{N})$ is not empty since the embedding $H^1(\mathbb{S}^1, \mathscr{N}) \hookrightarrow C^0(\mathbb{S}^1, \mathscr{N})$ is compact and dense. Then, notice the infimum in (1.2.6) is achieved, and all the minimizers c are geodesics. Thus, $|c'|$ is constant, and $\lambda(\gamma) = 2\pi\,|c'|$ coincides with the length of a minimizing geodesic.

In the definition of the energy cost of a defect, it is convenient take into account the product we have endowed $\Gamma(\mathscr{N})$ with. For each $\gamma \in \Gamma(\mathscr{N})$ we set

$$\lambda_*(\gamma) := \inf\left\{\frac{1}{4\pi}\sum_{i=1}^k \lambda^2(\gamma_i)\colon k \in \mathbb{N}, \ \gamma_i \in \Gamma(\mathscr{N}), \, \gamma \in \prod_{i=1}^k \gamma_i\right\}, \tag{1.2.7}$$

where the order of the product is not relevant. It is worth pointing out that the infimum in (1.2.7) is, in fact, a minimum. Indeed, since $\mathscr{N}$ is compact manifold, its fundamental group is finitely generated; on the other hand, γ contains only a finite number of elements of $\pi_1(\mathscr{N}, v_0)$, by (H_5). As a result, we see that the infimum in (1.2.7) is computed over finitely many k-uples $(\gamma_1, \ldots, \gamma_k)$.

Roughly speaking, the number $\lambda_*(\gamma)$ can be regarded as the energy cost of the defect γ. For example, when $\mathscr{N} = \mathbb{S}^1$ we have $\Gamma(\mathbb{S}^1) \simeq \pi_1(\mathbb{S}^1) \simeq \mathbb{Z}$, that is, the homotopy classes in $\Gamma(\mathbb{S}^1)$ are completely determined by their degree $d \in \mathbb{Z}$. Besides, $\lambda(d) = 2\pi\,|d|$ and $\lambda_*(d) = \pi\,|d|$, the infimum in (1.2.7) being reached by the decomposition

$$\gamma_1 = \gamma_2 = \cdots = \gamma_{|d|} = \operatorname{sign} d = \pm 1.$$

Hence, in this case decomposing the defect is energetically favorable. This is related to the quantization of singularities in the Ginzburg-Landau model (see [14]). By definition, λ_* enjoys the useful property

$$\lambda_*(\gamma) \leq \sum_{i=1}^k \lambda_*(\gamma_i) \qquad \text{if} \quad \gamma \in \prod_{i=1}^k \gamma_i \quad \text{with} \quad \gamma_i \in \Gamma(\mathscr{N}). \tag{1.2.8}$$

We conclude this subsection by coming back to Problem (P_ε) and fixing some notation that will be used throughout this work.

Definition 1.2.1. A continuous function $g\colon \partial\Omega \to \mathscr{N}$ will be called *homotopically trivial* if and only if it can be extended to a continuous function $\overline{\Omega} \to \mathscr{N}$, and homotopically non-trivial (or simply non-trivial) otherwise.

In case Ω is a simply connected domain, thus homeomorphic to a disk, being homotopically trivial is equivalent to being null-homotopic, that is, being homotopic to a constant. By contrast, these notions do not coincide any longer for a general domain. For instance, suppose that Ω is an annulus, bounded by two circles C_1 and C_2, and that g_1, g_2 are smooth data, defined on C_1, C_2 respectively and taking values in $\mathscr{N}$. If g_1, g_2 are in the same homotopy class, then the boundary datum is homotopically trivial in the sense of the previous definition, although each g_i, considered in itself, might not be null-homotopic. We will provide a characterization of homotopically trivial boundary data, for general domains, with the help of the tools we have described in this section.

Label the connected components of $\partial\Omega$ as $C_1, \ldots, C_k$, and denote by γ_i, for $i \in \{1, \ldots, k\}$, the free homotopy class of the boundary datum g restricted to C_i. Define

$$\kappa_* := \inf \left\{ \lambda_*(\gamma)\colon \gamma \in \prod_{i=0}^{k} \gamma_i \right\},$$

where λ_* has been introduced in (1.2.7). By definition of λ_*, we have

$$\kappa_* = \inf \left\{ \frac{1}{4\pi} \sum_{j=1}^{m} \lambda^2(\eta_j)\colon m \in \mathbb{N},\ \eta_j \in \Gamma(\mathscr{N}),\ \prod_{j=1}^{m} \eta_j \cap \prod_{i=1}^{k} \gamma_i \neq \emptyset \right\}. \tag{1.2.9}$$

In both formulae, the infima are taken over finite sets, and hence are minima.

As a straightforward consequence of Lemma 1.2.1, we obtain the following result, characterizing trivial boundary data. The proof is left to the reader.

Corollary 1.2.2. *Let $D \subseteq \mathbb{R}^2$ be a smooth, bounded domain, and let g_i, γ_i be as in Lemma 1.2.1. Then, the following conditions are equivalent:*

(i) the boundary datum $(g_i)_{i=1}^k$ is homotopically trivial;

(ii) denoting by ϵ the free homotopy class of any constant map in $\mathscr{N}$, we have

$$\epsilon \in \prod_{i=1}^{k} \gamma_i;$$

(iii) $\kappa_* = 0$.

1.2.2 The nearest point projection onto a manifold

In this subsection, we discuss briefly a geometric tool which will be exploited in our analysis: the nearest point projection on a manifold. Let $\mathscr{N}$ be a compact, smooth submanifold of $\mathbb{R}^d$, of dimension n and codimension k (that is, $d = n + k$). It is well known (see, for instance, [107, Chapter 3, p. 57]) that there exists a neighborhood U of $\mathscr{N}$ with the following property: for all $v \in U$, there exists a unique point $\pi(v) \in \mathscr{N}$ such that

$$|v - \pi(v)| = \mathrm{dist}(v,\, \mathscr{N}). \tag{1.2.10}$$

The mapping $v \in U \mapsto \pi(v)$ is called the *nearest point projection* (or simply projection, for short) onto $\mathscr{N}$. It is smooth, provided that U is small enough. Moreover, $v - \pi(v)$ is a normal vector to $\mathscr{N}$ at each point $v \in \mathscr{N}$ (all this facts are proved, e.g., in [107]). A neighborhood U of $\mathscr{N}$ such that π is defined and smooth on U is called a *tubular neighborhood.* Throughout this work, we assume that the δ_0-neighborhood of $\mathscr{N}$, where δ_0 is introduced in (H_2), is a tubular neighborhood.

Remark 1.2.4. With the help of π, we can easily derive from (H_2) some useful properties of f and its derivatives. Let $v \in \mathbb{R}^d$ be such that $\mathrm{dist}(v,\, \mathscr{N}) \leq \delta_0$. Then,

$$m_0 \,\mathrm{dist}(u,\, \mathscr{N}) \leq \mathrm{D}f(u) \cdot (u - \pi(u)) \leq M_0 \,\mathrm{dist}(u,\, \mathscr{N}).$$

The lower bound is given by (H_2), whereas the upper bound is obtained by a Taylor expansion of $\mathrm{D}f$ around the point $\pi(u)$ (remind that $\mathrm{D}f(\pi(u)) = 0$ because f is minimized on $\mathscr{N}$). As $\mathscr{N}$ is compact, the constant M_0 can be chosen independently of v. Via the fundamental theorem of calculus, we infer also

$$\frac{1}{2}m_0 \operatorname{dist}^2(u, \mathscr{N}) \leq f(u) = \int_0^1 \mathrm{D}f\left(\pi(u) + t(u - \pi(u))\right) \cdot (u - \pi(u))\,\mathrm{d}t \leq \frac{1}{2}M_0 \operatorname{dist}^2(u, \mathscr{N}).$$

The following lemma establishes a gradient estimate for the projection of mappings.

Lemma 1.2.3. *Let $u \in C^1(\Omega, \mathbb{R}^d)$ be such that $\operatorname{dist}(u(x), \mathscr{N}) \leq \delta_0$ for all $x \in \Omega$, and define*

$$\sigma(x) := \operatorname{dist}(u(x), \mathscr{N}), \qquad v(x) := \pi(u(x))$$

for all $x \in \Omega$. Then, the estimates

$$(1 - M\sigma)\left|\nabla v\right|^2 \leq \left|\nabla u\right|^2 \leq (1 + M\sigma)\left|\nabla v\right|^2 + \left|\nabla\sigma\right|^2 \tag{1.2.11}$$

hold, for a constant M depending only on $\mathscr{N}$, k.

Proof. Fix a point $x \in \Omega$. Let $\nu_1, \nu_2, \ldots, \nu_k$ be a moving orthonormal frame for the normal space to $\mathscr{N}$, defined on a neighborhood of $v(x)$. (Even if $\mathscr{N}$ is not orientable, such a frame is locally well-defined). Then, for all y in a neighborhood of x, there exist some numbers $\alpha_1(y), \alpha_2(y), \ldots, \alpha_k(y)$ such that

$$u(y) = v(y) + \sum_{i=1}^k \alpha_i(y)\nu_i(v(y)). \tag{1.2.12}$$

The functions v, α_i are as regular as u. Differentiating the equation (1.2.12), and raising to the square each side of the equality, we obtain

$$\begin{aligned}\left|\nabla u\right|^2 - \left|\nabla v\right|^2 = \sum_{i=1}^k \Big\{ &\alpha_i^2 \left|\nabla\nu_i(v)\right|^2 + \left|\nabla\alpha_i\right|^2 \\ &+ 2\alpha_i\nabla v : \nabla\nu_i(v) + 2\nabla v : (\nu_i(v) \otimes \nabla\alpha_i) + 2\alpha_i\nabla\nu_i(v) : (\nu_i(v) \otimes \nabla\alpha_i) \Big\}.\end{aligned} \tag{1.2.13}$$

The fourth term in the right-hand side vanishes, because ∇v is tangent to $\mathscr{N}$. The last term vanishes as well since, differentiating $\nu_i = 1$, we have $(\nabla\nu_i)\nu_i = 0$. For the first term of the right-hand side, we set

$$M := 1 + \sup_{1 \leq i \leq k} \left\|\nabla\nu_i\right\|^2_{L^\infty}$$

and we remark that

$$\sum_{i=1}^k \alpha_i^2 \left|\nabla\nu_i(v)\right|^2 \leq M \sum_{i=1}^k \alpha_i^2 \left|\nabla v\right|^2 = M\sigma^2 \left|\nabla v\right|^2.$$

By the Cauchy-Schwarz inequality and $\sum_{i=1}^k \alpha_i \leq C_k \left(\sum_{i=1}^k \alpha_i^2\right)^{1/2}$, we can write

$$\left|\sum_{i=1}^k \alpha_i \nabla v : \nabla\nu_i(v)\right| \leq M \sum_{i=1}^k \alpha_i \left|\nabla v\right|^2 \leq M\sigma \left|\nabla v\right|^2, \tag{1.2.14}$$

up to modifying the value of M in order to absorb the factor C_k. Furthermore, since $\sigma \leq \delta_0 < 1$, from (1.2.13) and (1.2.14) we infer

$$(1 - M\sigma)\left|\nabla v\right|^2 + \sum_{i=1}^k \left|\nabla\alpha_i\right|^2 \leq \left|\nabla u\right|^2 \leq (1 + M\sigma)\left|\nabla v\right|^2 + \sum_{i=1}^k \left|\nabla\alpha_i\right|^2. \tag{1.2.15}$$

The lower bound in (1.2.11) follows immediately, and we only need to estimate the derivatives of α_i to conclude. It follows from (1.2.12) that $\alpha_i = (u - v) \cdot \nu_i(v)$. Differentiating and raising to the square this identity, and taking into account that $(\nabla\nu_i)\nu_i = 0$, we deduce

$$\sum_{i=1}^{k} |\nabla\alpha_i|^2 = \sum_{i=1}^{k} \left\{ |\nabla(u - v) \cdot \nu_i(v)|^2 + |(u - v) \cdot \nabla\nu_i(v)|^2 \right\}.$$

Then

$$\sum_{i=1}^{k} |\nabla\alpha_i|^2 \leq M \left\{ |\nabla(u - v)|^2 + \sigma^2 |\nabla v|^2 \right\}. \tag{1.2.16}$$

Computing the gradient of $\sigma = |u - v|$ by the chain rule yields $|\nabla\sigma| = |\nabla(u - v)|$. Therefore, the estimates (1.2.14) and (1.2.16) imply the upper bound in (1.2.11).

Notice that our choice of the constant M depends on the neighborhood where the frame $(\nu_i)_{1\leq i\leq k}$ is defined. However, since $\mathscr{N}$ is compact, we can find a constant for which the inequality (1.2.11) holds globally. □

1.3 Biaxiality in the Landau-de Gennes model

We focus here on the Landau-de Gennes model (LG$_\varepsilon$). To stress that this discussion pertains to a specific case, throughout the section we use Q instead of u as the variable in the target space, and use Q_ε (instead of u_ε) to denote minimizers. The aim of this section is to prove Theorem 1.1.1.

1.3.1 On the structure of the Q-tensors space

We discuss here general facts about Q-tensors, which are useful in order to to have an insight into the structure of the target space $\mathbf{S}_0$. The starting point of our analysis is the following representation formula. Slightly different forms of this formula are often found in the literature (e.g. [98, Proposition 1]).

Lemma 1.3.1. *For all fixed $Q \in \mathbf{S}_0 \setminus \{0\}$, there exist two numbers $s \in (0, +\infty)$, $r \in [0, 1]$ and an orthonormal pair of vectors $(\mathbf{n}, \mathbf{m})$ in $\mathbb{R}^3$ such that*

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) + sr\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right). \tag{1.3.1}$$

Given Q, the parameters $s = s(Q)$, $r = r(Q)$ are uniquely determined. The functions $Q \mapsto s(Q)$ and $Q \mapsto r(Q)$ are locally Lipschitz-continuous on $\mathbf{S}_0 \setminus \{0\}$ and positively homogeneous of degree 1 and 0, respectively.

Sketch of the proof. Label the eigenvalues of Q as $\lambda_1 \geq \lambda_2 \geq \lambda_3$. Let $(s, r, \mathbf{n}, \mathbf{m})$ be a set of parameters with the desired properties, and let $\mathbf{p} := \mathbf{n} \times \mathbf{m}$, so that $(\mathbf{n}, \mathbf{m}, \mathbf{p})$ is a positive orthonormal basis of $\mathbb{R}^3$. Thanks to the identity $\mathrm{Id} = \mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2} + \mathbf{p}^{\otimes 2}$, we can rewrite (1.3.1) as

$$Q = \frac{s}{3}(2 - r)\mathbf{n}^{\otimes 2} + \frac{s}{3}(r - 1)\mathbf{m}^{\otimes 2} - \frac{s}{3}(1 + r)\mathbf{p}^{\otimes 2}.$$

The constraints $s \geq 0$, $0 \leq r \leq 1$ entail

$$\frac{s}{3}(2 - r) \geq \frac{s}{3}(r - 1) \geq -\frac{s}{3}(1 + r).$$

We conclude that

$$\lambda_1 = \frac{s}{3}(2 - r), \qquad \lambda_2 = \frac{s}{3}(r - 1), \qquad \lambda_3 = -\frac{s}{3}(1 + r),$$

and that $\mathbf{n}$, $\mathbf{m}$, $\mathbf{p}$ are eigenvectors associated with λ_1, λ_2, λ_3 respectively. By straightforward computations, it follows that

$$s(Q) = 2\lambda_1 + \lambda_2, \qquad r(Q) = \frac{\lambda_1 + 2\lambda_2}{2\lambda_1 + \lambda_2}. \tag{1.3.2}$$

Then, it is clear that s and r are positively homogeneous of degree 1, 0 respectively, whereas the local Lipschitz continuity follows by standard regularity results for the eigenvalues(see, e.g. [8, Section 9.1] implies that s, r are continuous. Conversely, it is easily checked that (s, r) defined by (1.3.2), together with an orthonormal pair of eigenvectors $(\mathbf{n}, \mathbf{m})$ relative to (λ_1, λ_2), satisfy (1.3.1). □

Remark 1.3.1. The classification of Q-tensors can be reformulated in terms of s, r.

- The isotropic state $Q = 0$ correspond to $s(Q) = 0$.
- A matrix $Q \in \mathbf{S}_0$ is uniaxial if and only if $s(Q) > 0$ and $r(Q) \in \{0, 1\}$. More precisely, $r(Q) = 0$ if and only if the leading eigenvalue λ_1 is simple and $\lambda_2 = \lambda_3$ (these are *prolate uniaxial* matrices). On the other hand, $r(Q) = 1$ if and only if $\lambda_1 = \lambda_2$ and the least eigenvalue λ_3 is simple (*oblate uniaxial* matrices).
- A matrix $Q \in \mathbf{S}_0$ is biaxial if and only if $s(Q) > 0$ and $0 < r(Q) < 1$.

Taking advantage of Lemma 1.3.1, we give the proof of a property we have claimed in the Introduction of this thesis, which allows to interpret Q as a renormalized second order moment of a probability distribution on the unit sphere. Let μ be a probability measure on $\mathscr{B}(\mathbb{S}^2)$, satisfying

$$\mu(B) = \mu(-B) \qquad \text{for every } B \in \mathscr{B}(\mathbb{S}^2). \tag{1.3.3}$$

Physically, $\mu(B)$ represents the proportion of molecules oriented along a direction contained in B, at a point $x \in \Omega$. If μ is the uniform distribution, that is

$$\mu = \mu_0 := \frac{1}{4\pi}\mathscr{H}^2 \llcorner \mathbb{S}^2,$$

then we say that μ is isotropic. We say that μ is uniaxial if and only if μ has an axis of rotational symmetry, that is there exists $\mathbf{n} \in \mathbb{S}^2$ such that, for any rotation $R \in \mathrm{SO}(3)$ satisfying $R\mathbf{n} = \mathbf{n}$, there holds

$$\mu(R(B)) = \mu(B) \qquad \text{for any } B \in \mathscr{B}(\mathbb{S}^2).$$

We say that μ is biaxial if and only if there exists an orthogonal frame $(\mathbf{n}, \mathbf{m}, \mathbf{p})$ such that, for any reflection symmetry $S \in \mathrm{SO}(3)$ along one of the axes $\mathbf{n}$, $\mathbf{m}$ or $\mathbf{p}$, there holds

$$\mu(S(B)) = \mu(B) \qquad \text{for any } B \in \mathscr{B}(\mathbb{S}^2).$$

Lemma 1.3.2. *Let $Q \in \mathbf{S}_0$ be a given tensor, satisfying the eigenvalue constraint*

$$-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3} \qquad \text{for } i \in \{1, 2, 3\}. \tag{1.3.4}$$

Then, there exists a probability measure μ on $\mathscr{B}(\mathbb{S}^2)$ which satisfies (1.3.3)*,*

$$Q = \int_{\mathbb{S}^2} \left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) \mathrm{d}\mu(\mathbf{p}) \tag{1.3.5}$$

and is uniaxial (respectively, biaxial, isotropic) if Q is uniaxial (biaxial, isotropic).

Proof. In view of the representation formula of Lemma 1.3.1, it suffices to consider a uniaxial matrix Q. Then, the case of a biaxial matrix will follow by additivity. Moreover, up to a rotation we can assume that $\mathbf{n} = \mathbf{e}_3$. Therefore, without loss of generality we assume that

$$Q = s\left(\mathbf{e}_3^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{for some } s \geq 0.$$

Then, the eigenvalue constraint (1.3.4) reduces to $0 \leq s \leq 1$. If $s = 1$, the measure $\mu = (\delta_{\mathbf{e}_3} + \delta_{-\mathbf{e}_3})/2$ satisfies to all the desired properties. On the other hand, if $s = 0$ then $Q = 0$ and the lemma follows by taking $\mu = \mu_0$. We consider now the case $0 < s < 1$. Using spherical coordinates $(\theta,\, \varphi) \in (0,\, \pi) \times (0,\, 2\pi)$, we make the ansatz

$$\mu = h(\theta) \sin\theta \,\mathrm{d}\theta \,\mathrm{d}\varphi$$

where $h\colon (0,\, \pi) \to \mathbb{R}$ is a measurable positive function, which satisfies to

$$\int_0^\pi h(\theta)\sin\theta\,\mathrm{d}\theta = \frac{1}{2\pi} \tag{1.3.6}$$

and

$$h(\theta) = h(\pi - \theta) \qquad \text{for any } \theta \in (0,\, \pi). \tag{1.3.7}$$

Any such measure μ is a probability measure on the unit sphere and satisfies (1.3.3). Before injecting this ansatz into Equation (1.3.5), we compute

$$\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} = \begin{pmatrix} \sin^2\theta\cos^2\varphi - \frac{1}{3} & \sin^2\theta\cos\varphi\sin\varphi & \sin\theta\cos\theta\cos\varphi \\ \sin^2\theta\cos\varphi\sin\varphi & \sin^2\theta\sin^2\varphi - \frac{1}{3} & \sin\theta\cos\theta\sin\varphi \\ \sin\theta\cos\theta\cos\varphi & \sin\theta\cos\theta\sin\varphi & \frac{2}{3} - \sin^2\theta \end{pmatrix}.$$

The integral of the off-diagonal components with respect to $\varphi \in (0,\, 2\pi)$ vanish. By computing explicitly, one sees that (1.3.5) is equivalent to

$$\int_0^\pi \left(\frac{2}{3} - \sin^2\theta\right) h(\theta)\sin\theta\,\mathrm{d}\theta = \frac{s}{3\pi}$$

or also, taking (1.3.6) into account,

$$\int_0^\pi h(\theta)\sin^3\theta\,\mathrm{d}\theta = \frac{1-s}{3\pi}. \tag{1.3.8}$$

At the end of the day, we look for a positive function $h\colon (0,\, \pi) \to \mathbb{R}$ which satisfies (1.3.6), (1.3.7) and (1.3.8). We take h of the form

$$h(\theta) := \frac{\alpha\beta}{\alpha^2 + \cos^2\theta},$$

for some positive parameters α, β, so (1.3.7) is satisfied. We have

$$\int_0^\pi h(\theta)\sin\theta\,\mathrm{d}\theta = 2\alpha\beta\int_0^1 \frac{\mathrm{d}t}{\alpha^2 + t^2} = 2\beta\arctan\left(\frac{1}{\alpha}\right)$$

and we choose

$$\beta := \left(4\pi\arctan\left(\frac{1}{\alpha}\right)\right)^{-1},$$

so Condition (1.3.6) is satisfied too. Finally,

$$\int_0^\pi h(\theta)\sin^3\theta\,\mathrm{d}\theta = 2\alpha\beta\int_0^1 \frac{1-t^2}{\alpha^2+t^2}\,\mathrm{d}t = \frac{1}{2\pi} - \frac{\alpha}{2\pi\arctan(1/\alpha)} + \frac{\alpha^2}{2\pi}.$$

The right-hand side is a continuous function of α on $(0,\, +\infty)$, which tends to $(2\pi)^{-1}$ as $\alpha \to 0^+$ and to 0 as $\alpha \to +\infty$. In particular, the image of this function contains the whole interval $(0,\, (3\pi)^{-1})$. Therefore, for any $0 < s < 1$ there exists $\alpha > 0$ so that (1.3.8) is satisfied. $\square$

We introduce now a few objects, which are helpful in the description of the Q-tensor space $\mathbf{S}_0$. first of all, we recall the definition of the *biaxiality parameter* of a matrix Q:

$$\beta(Q) := 1 - 6\frac{\left(\operatorname{tr} Q^3\right)^2}{\left(\operatorname{tr} Q^2\right)^3} \qquad \text{for } Q \in \mathbf{S}_0 \setminus \{0\}. \tag{1.3.9}$$

This defines a homogeneous function of Q such that $0 \leq \beta(Q) \leq 1$, with $\beta(Q) = 0$ if and only if Q is uniaxial, and $\beta(Q) = 1$ if and only if $\det Q = 0$ (see, for instance, [98, Lemma 1 and Appendix] and the references therein). We say that a measurable map $Q\colon \Omega \to \mathbf{S}_0$ is *maximally biaxial* if and only if

$$\operatorname{ess\,sup}_\Omega \beta(Q) = 1.$$

The biaxiality parameter can be written as a function of $r(Q)$:

$$\beta(Q) = \frac{27 r^2(Q)\left(1 - r(Q)\right)^2}{4\left(r^2(Q) - r(Q) + 1\right)}$$

(compare, for instance, [98, Equation (187)]). In particular, we have

$$\beta(Q) = 1 \qquad \text{if and only if} \qquad r(Q) = \frac{1}{2}. \tag{1.3.10}$$

Note that the modulus of a matrix $|Q|$ can be written as a function of $s(Q)$, $r(Q)$ as well:

$$|Q|^2 = \frac{2}{3} s^2(Q)\left(r^2(Q) - r(Q) + 1\right). \tag{1.3.11}$$

This follows from Lemma 1.3.1, in a straightforward way.

Another key object in our analysis will be the vacuum manifold $\mathscr{N}$, i.e. set of minimizers of the Landau-de Gennes potential f. With the help of Lemma 1.3.1, the set $\mathscr{N}$ can be described as follows.

Proposition 1.3.3. *Let the potential f be given by* (1.1.2)*, where the constant k_0 is chosen in such a way that* $\inf f = 0$*, and set $\mathscr{N} := f^{-1}(0)$. Then,*

$$\mathscr{N} = \left\{ s_* \left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\operatorname{Id} \right) : \mathbf{n} \in \mathbb{S}^2 \right\},$$

where

$$s_* := s_*(a,\, b,\, c) = \frac{1}{4c}\left\{ b + \sqrt{b^2 + 24ac} \right\}. \tag{1.3.12}$$

The set $\mathscr{N}$ is a smooth submanifold of $\mathbf{S}_0$, diffeomorphic to the projective plane $\mathbb{RP}^2$, and any matrix $Q \in \mathscr{N}$ satisfies

$$|Q| = s_* \sqrt{\frac{2}{3}}, \qquad \beta(Q) = 0.$$

The reader is referred to [98, Propositions 9 and 15] for the proof. Here, we mention only that the existence of a diffeomorphism $\mathbb{RP}^2 \to \mathscr{N}$ is immediately clear, if we identify the projective space with a set of matrices as we did in the introduction of this thesis. Proposition 1.3.3 implies that

$$\pi_1(\mathscr{N}) \simeq \mathbb{Z}/2\mathbb{Z},$$

so the assumption (H_5) is satisfied. For future reference, we also note that the universal covering $\mathbb{S}^2 \to \mathscr{N}$ is realized by the smooth map

$$\psi\colon \mathbf{n} \in \mathbb{S}^2 \mapsto s_* \left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\operatorname{Id} \right). \tag{1.3.13}$$

This map is onto and satisfies $\psi(\mathbf{n}) = \psi(-\mathbf{n})$, for any $\mathbf{n} \in \mathbb{S}^2$. Moreover, there exists a covering of $\mathbb{RP}^2$ with open sets $U \subseteq \mathbb{RP}^2$, such that the inverse image of any such U is the disjoint union of two open sets V_1, $V_2 \subseteq \mathbb{S}^2$, and ψ restricts to homeomorphisms $\phi_{|U_i} \colon U_i \to V$ for $i \in \{1, 2\}$. As we will see in a moment, this map has other nice local properties, which can be exploited to compute the number κ_* associated with $\mathscr{N}$. Note that, since $\Gamma(\mathscr{N})$ contains exactly two elements, Equation (1.2.9) which defines κ_* reduces to

$$\kappa_* = \inf\left\{\frac{1}{2}\int_{\mathbb{S}^1} \left|P'(\theta)\right|^2 \,\mathrm{d}\theta \colon P \in H^1(\mathbb{S}^1, \mathscr{N}) \text{ is homotopically non-trivial}\right\}. \tag{1.3.14}$$

Lemma 1.3.4. *We have*

$$\kappa_* = \frac{\pi}{2} s_*^2$$

and a minimizer for (1.3.14) *is given by*

$$P(\theta) := s_*\left(\mathbf{n}_*^{\otimes 2}(\theta) - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{for } 0 \leq \theta \leq 2\pi,$$

where $\mathbf{n}_*(\theta) = (\cos(\theta/2),\, \sin(\theta/2),\, 0)^\mathsf{T}$.

Proof. Fix $\mathbf{n} \in \mathbb{S}^2$ and a tangent vector $\mathbf{v} \in T_n\mathbb{S}^2$. By differentiating the function $t \mapsto \psi(\mathbf{n} + t\mathbf{v})$, we obtain

$$\langle \mathrm{d}\psi(\mathbf{n}),\, \mathbf{v}\rangle = s_*\left(\mathbf{n} \otimes \mathbf{v} + \mathbf{v} \otimes \mathbf{n}\right),$$

and it follows that

$$\left|\langle \mathrm{d}\psi(\mathbf{n}),\, \mathbf{v}\rangle\right|^2 = 2s_*^2 \sum_{i,\, j} \left(\mathbf{n}_i\mathbf{v}_j\mathbf{n}_i\mathbf{v}_j + \mathbf{n}_i\mathbf{v}_j\mathbf{v}_i\mathbf{n}_j\right) = 2s_*^2 \left|\mathbf{v}\right|^2. \tag{1.3.15}$$

Denote by g, h the first fundamental forms on $\mathbb{S}^2$, $\mathscr{N}$ respectively (that is, the restriction of the euclidean scalar products of $\mathbb{R}^3$, $\mathbf{S}_0$ to the tangent planes of $\mathbb{S}^2 \subseteq \mathbb{R}^3$ $\mathscr{N} \subseteq \mathbf{S}_0$). In terms of pull-back metrics, Equation (1.3.15) gives

$$\psi^* h = 2s_*^2 g.$$

The scaling factor $2s_*^2$ is constant, so the Levi-Civita connections associated with ψ^*h and g coincide, for the Christoffel symbols

$$\Gamma^i_{jk} = \frac{1}{2} g^{il}\left(\frac{\partial g_{lj}}{\partial x^k} + \frac{\partial g_{lk}}{\partial x^j} - \frac{\partial g_{jk}}{\partial x^l}\right)$$

of the two metrics coincide. As a consequence, a loop P is a geodesic in $\mathscr{N}$ if and only if it can be written as $P = \psi \circ \mathbf{n}$, where $\mathbf{n} \colon [0, 2\pi] \to \mathbb{S}^2$ is a geodesic path in $\mathbb{S}^2$.

Let $\mathbf{n} \colon [0,\, 2\pi] \to \mathbb{S}^2$ be a geodesic path, that is, an arc of great circle. The map $P := \psi \circ \mathbf{n}$ is a loop if and only if $\psi(\mathbf{n}(0)) = \psi(\mathbf{n}(1))$, which means either $\mathbf{n}(0) = \mathbf{n}(1)$ or $\mathbf{n}(0) = -\mathbf{n}(1)$. In the first case, P is homotopically trivial in $\mathscr{N}$. In the second case, P is a non-trivial geodesic loop, and its homotopy class generates the fundamental group $\pi_1(\mathscr{N})$. Since there are no other geodesic loops in $\mathscr{N}$, we deduce that any minimizer for (1.2.9) must be of the form $P = \psi \circ \mathbf{n}$, where $\mathbf{n}$ is half of a great circle in $\mathbb{S}^2$ parametrized by multiples of arc-length. Now the lemma follows from easy computations. ☐

There is another set which is important for our analysis, namely

$$\mathscr{C} := \left\{Q \in \mathbf{S}_0 \setminus \{0\} \colon r(Q) = 1\right\} \cup \{0\}.$$

This is a closed subset of $\mathscr{C}$, and it is cone (i.e., $\lambda Q \in \mathscr{C}$ for any $Q \in \mathscr{C}$, $\lambda \in \mathbb{R}^+$). In view of (1.3.2), we have

$$\mathscr{C} = \left\{Q \in \mathbf{S}_0 \colon \lambda_1(Q) = \lambda_2(Q)\right\},$$

i.e. $\mathscr{C}$ is the set of matrices whose leading eigenvalue has multiplicity > 1 (oblate uniaxial matrices). As a consequence, $Q_0 \in \mathscr{C}$ if and only if a map $Q \mapsto \mathbf{n}(Q)$, where $\mathbf{n}(Q)$ is a unit eigenvector associated with $\lambda_1(Q)$, *fails* to be continuously defined in a neighborhood of Q_0 (see e.g. [8, Section 9.1, Equation (9.1.41), p. 600]). As we will see in a moment, this fact has remarkable consequences on the topological structure of $\mathbf{S}_0$.

Lemma 1.3.5. *$\mathscr{C} \setminus \{0\}$ is diffeomorphic to $\mathbb{RP}^2 \times \mathbb{R}$.*

Proof. As we did in the introduction of this thesis, we identify $\mathbb{RP}^2$ with a set of matrices. Using Lemma 1.3.1, we can write any $Q \in \mathscr{C} \setminus \{0\}$ in the form

$$Q = s\left(\mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2} - \frac{2}{3}\,\mathrm{Id}\right)$$

for some orthonormal couple of vectors $\mathbf{n},\, \mathbf{m} \in \mathbb{R}^3$. Set $\mathbf{p} = \mathbf{n} \times \mathbf{m}$, so that $(\mathbf{n},\, \mathbf{m},\, \mathbf{p})$ is an orthonormal, positively oriented basis in $\mathbb{R}^3$. Using the identity $\mathrm{Id} = \mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2} + \mathbf{p}^{\otimes 2}$, we compute

$$Q = -s\left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right). \tag{1.3.16}$$

The eigenvalues of Q, counted with their multiplicity, are $(s/3,\, s/3,\, -2s/3)$, and $\mathbf{p}$ is an eigenvector corresponding to the negative eigenvalue.

In view of (1.3.16), it is natural to define a map $\varphi\colon \mathscr{C} \setminus \{0\} \to \mathbb{RP}^2 \times (0,\, +\infty)$ as follows. For a given $Q \in \mathscr{C} \setminus \{0\}$, let $\mathbf{p}$ be a unit eigenvector corresponding to the negative eigenvalue ($\mathbf{p}$ is well-defined up to a sign). Then, set

$$\varphi(Q) := \left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id},\, s(Q)\right).$$

This function is well-defined and continuous (because the negative eigenvalue of Q has multiplicity 1, we can apply standard continuity results for the eigenvectors, e.g. [8, Section 9.1 and in particular (9.1.41), p. 600]). The map

$$(P,\, s) \in \mathbb{RP}^2 \times (0,\, +\infty) \mapsto -sP \in \mathscr{C} \setminus \{0\}$$

is also continuous, and is readily checked to be an inverse for φ. Therefore, φ provides the desired homeomorphism. ☐

The importance of $\mathscr{C}$ is explained by the following lemma.

Lemma 1.3.6. *The set $\mathbf{S}_0 \setminus \mathscr{C}$ retracts (by deformation) on $\mathscr{N}$.*

Proof. To construct a retraction, we exploit the representation formula of Lemma 1.3.1, and define the functions $K,\, H\colon \mathbf{S}_0 \setminus \mathscr{C} \times [0,\, 1] \to \mathbf{S}_0$ by

$$K(P,\, t) := \mathbf{n}^{\otimes 2}(P) - \frac{1}{3}\,\mathrm{Id} + t\, r(P)\left(\mathbf{m}^{\otimes 2}(P) - \frac{1}{3}\,\mathrm{Id}\right)$$

and

$$H(P,\, t) := (t\, s(P) + (1-t)s_*)\, K(P,\, t).$$

The homogeneity of r implies that

$$r\left(K(P,\, t)\right) = r\left(H(P,\, t)\right) = tr(P) < 1,$$

so $H(P,\, t) \notin \mathscr{C} \setminus \mathbf{S}_0$ for all $(P,\, t) \in (\mathbf{S}_0 \setminus \mathscr{C}) \times [0,\, 1]$. By Lemma (1.3.1), the mapping $P \mapsto (s(P),\, r(P))$ is continuous on $\mathbf{S}_0 \setminus \mathscr{C}$. As a consequence, H is well-defined and continuous, if K is. Moreover, H enjoys these properties: for all $P \in \mathbf{S}_0 \setminus \mathscr{C}$, we have $H(P,\, 1) = P$ and $H(P,\, 0) \in \mathscr{N}$, whereas $H(P,\, t) = P$

for all $(P, t) \in \mathscr{N} \times [0, 1]$. To conclude that H is a retraction by deformation, it only remains to check that K is well-defined and continuous.

Remark that each $P \in \mathbf{S}_0 \setminus \mathscr{C}$ has the leading eigenvalue of multiplicity one, so $\mathbf{n} = \mathbf{n}(P)$ is uniquely determined, up to a sign, and $\mathbf{n}^{\otimes 2}$ is well-defined. In case $r = r(P) \neq 0$, the second eigenvalue is simple as well, and the same remark applies to $\mathbf{m}$. If $r(P) = 0$ then $K(P, t)$ is equally well-defined, regardless of the choice of $\mathbf{m}$.

We argue somehow similarly for the continuity. If $\{(P_k, t_k)\}_{k\in\mathbb{N}}$ is a sequence in $(\mathbf{S}_0 \setminus \mathscr{C}) \times [0, 1]$ converging to $(P, t) \in (\mathbf{S}_0 \setminus \mathscr{C}) \times [0, 1]$, then

$$\begin{aligned}|K(P_k, t_k) - K(P, t)| \leq &\left|\mathbf{n}^{\otimes 2}(P_k) - \mathbf{n}^{\otimes 2}(P)\right| + |t_k - t|\, r(P_k) \left|\mathbf{m}^{\otimes 2}(P_k) - \frac{1}{3}\,\mathrm{Id}\right| \\ &+ t\left|r(P_k)\mathbf{m}^{\otimes 2}(P_k) - r(P)\mathbf{m}^{\otimes 2}(P)\right| + t\,|r(P_k) - r(P)|\,.\end{aligned}$$

As the leading eigenvalue of $P \in \mathbf{S}_0 \setminus \mathscr{C}$ is simple, standard results about the continuity of eigenvectors (see, for instance, [8, Equation (9.1.41), p. 600]) imply that $\mathbf{n}^{\otimes 2}(P_k) \to \mathbf{n}^{\otimes 2}(P)$. If $r(P) = 0$, this is enough to conclude, since

$$|K(P_k, t_k) - K(P, t)| \leq tr(P_k)\left|\mathbf{m}^{\otimes 2}(P_k)\right| + \mathrm{o}(1) \to tr(Q) = 0$$

as $k \to +\infty$. On the other hand, if $r(P) \neq 0$, then all the eigenvalues of P are simple, and hence $\mathbf{m}^{\otimes 2}(P_k) \to \mathbf{m}^{\otimes 2}(P)$ by the continuity results of [8] again. Therefore, K is continuous and $\mathbf{S}_0 \setminus \mathscr{C}$ retracts by deformation on $\mathscr{N}$. ☐

Throughout this chapter, we denote by $\mathscr{R} := H(\cdot, 0)\colon \mathbf{S}_0 \setminus \mathscr{C} \to \mathscr{N}$ the retraction constructed in Lemma 1.3.6.

Lemma 1.3.7. *The retraction $\mathscr{R}$ is of class C^1 on $\mathbf{S}_0 \setminus \mathscr{C}$.*

Proof. Fix a matrix $Q \in \mathbf{S}_0 \setminus \mathscr{C}$, and label $\lambda_1(Q) \geq \lambda_2(Q) \geq \lambda_3(Q)$ the eigenvalues of Q. The leading eigenvalue $\lambda_1(Q)$ is simple, because $r(Q) \neq 1$ implies $\lambda_1(Q) \neq \lambda_2(Q)$ by (1.3.2). Then, classical differentiability results for the eigenvectors (see e.g. [8]) imply that there exist a C^1 map $\mathbf{n}$, defined on a neighborhood of Q, such that $\mathbf{n}(P)$ is a unit eigenvector associated with the leading eigenvalue $\lambda_1(P)$, for any P close enough to Q. As a consequence, the map

$$\mathscr{R}(P) = s_*\left(\mathbf{n}^{\otimes 2}(P) - \frac{1}{3}\,\mathrm{Id}\right)$$

is of class C^1 in a neighborhood of Q. ☐

Remark 1.3.2. Take a continuous, non-trivial loop $Q\colon \mathbb{S}^1 \to \mathscr{N}$. Then, for any continuous extension $\tilde{Q}\colon B^2_1 \to \mathbf{S}_0$ of Q there exists a point $x_0 \in B^2_1$ such that $\tilde{Q}(x_0) \in \mathscr{C}$, otherwise composing with the retraction $\mathscr{R}$ would give a continuous map $B^2_1 \to \mathscr{N}$, which is impossible because Q is non-trivial. In this sense, the condition $\tilde{Q} \in \mathscr{C}$ identify the regions where topological defect occurs. Moreover, the cone $\mathscr{C}$ is a singular manifold of codimension two in $\mathbf{S}_0$, since $\mathscr{C} \setminus \{0\} \simeq \mathbb{RP}^2 \times \mathbb{R}$ by Lemma 1.3.5. Therefore, heuristically speaking, we expect $\tilde{Q}^{-1}(\mathscr{C})$ to be a set of codimension two for any $\tilde{Q} \in C^1(\Omega, \mathbf{S}_0)$.

We conclude this discussion with some properties of the Landau-de Gennes potential. In particular, we prove that this potential satisfies the assumptions (H_1)–(H_3), so the asymptotic analysis we carry out applies.

Lemma 1.3.8. *The potential f defined by* (1.2.2) *fulfills (H_1)–(H_3).*

Proof. We know by Proposition 1.3.3 that (H_1) is satisfied. With the help of Remark 1.2.2, we show that (H_3) is fulfilled as well. Indeed, we compute the gradient of f:

$$\mathrm{D}f(Q) = -aQ - bQ^2 - \frac{1}{3}b(\operatorname{tr} Q^2)\,\mathrm{Id} + cQ\operatorname{tr} Q^2$$

(we have taken into account the Lagrange multiplier associated with the tracelessness constraint). The inequality $\sqrt{6}\operatorname{tr} Q^3 \leq |Q|^3$ implies

$$\mathrm{D}f(Q)\cdot Q = -a\,|Q|^2 - b\operatorname{tr} Q^3 + c\,|Q|^4 \geq -a\,|Q|^2 - \frac{b}{\sqrt{6}}\,|Q|^3 + c\,|Q|^4\,,$$

and it is readily seen that the right-hand side is positive when $|Q|^2 > 2s_*^2/3$.

Finally, let us check the condition (H_2). For a fixed $Q \in \mathscr{N}$, there exists $\mathbf{n} \in \mathbb{S}^2$ such that $Q = \psi(\mathbf{n})$, where ψ is the smooth mapping defined by (1.3.13). Up to rotating the coordinate frame, we can assume without loss of generality that $\mathbf{n} = \mathbf{e}_3$. Because of (1.3.15), the tangent plane $T_Q\mathscr{N}$ is spanned by the matrices

$$X_k = \sqrt{\frac{3}{2}}(\mathbf{e}_k \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{e}_k), \qquad k \in \{1,\, 2\}.$$

As a consequence, $P \in \mathbf{S}_0$ is a normal vector to $\mathscr{N}$ at Q if and only if $P\cdot X_1 = P\cdot X_2 = 0$ or, equivalently, if and only if it can be written as

$$P = \begin{pmatrix} -\dfrac{p_1}{3} + p_3 & p_2 & 0 \\ p_2 & -\dfrac{p_1}{3} - p_3 & 0 \\ 0 & 0 & \dfrac{2p_1}{3} \end{pmatrix} \tag{1.3.17}$$

for some $(p_1,\, p_2,\, p_3) \in \mathbb{R}^3$. It is easily checked that $PQ = QP$. Now, we compute

$$\begin{aligned} \mathrm{D}f(Q+tP)\cdot P &= -a(Q+tP)\cdot P - b(Q+tP)^2\cdot P + c\operatorname{tr}(Q+tP)^2(Q+tP)\cdot P \\ &= t\left\{-a|P|^2 - 2b(PQ)\cdot P + 2c(\operatorname{tr} PQ)^2 + \frac{2}{3}s_*^2c|P|^2\right\} + O(t^2) \end{aligned}$$

(here we have used that $\mathrm{D}f(Q) = 0$). By (1.3.17), we have

$$|P|^2 = \frac{2}{3}p_1^2 + 2p_2^2 + 2p_3^2, \qquad \operatorname{tr} PQ = \frac{2}{3}s_*p_1, \qquad (PQ)\cdot P = \frac{2}{9}s_*\left(p_1^2 - 3p_2^2 - 3p_3^2\right)$$

and hence

$$\mathrm{D}f(Q+tP)\cdot P \geq t\left\{\frac{2}{3}\left(-a - \frac{2}{3}bs_* + 2cs_*^2\right)p_1^2 + 2\left(-a + \frac{2}{3}bs_* + \frac{2}{3}cs_*^2\right)(p_2^2 + p_3^2)\right\} + O(t^2).$$

The coefficients in the right-hand side are readily shown to be non negative, for the definition of s_* (Equation (1.3.12)) implies the identities

$$-a - \frac{2}{3}bs_* + 2cs_*^2 = \frac{1}{3}bs_* + 2a, \qquad -a + \frac{2}{3}bs_* + \frac{2}{3}cs_*^2 = bs_*.$$

Thus, we have proved that $\partial_P^2 f(Q) > 0$, with a uniform bound in $Q \in \mathscr{N}$. □

1.3.2 The energy functional in the low temperature regime

Before giving the proof of Theorem 1.1.1, it is convenient to rescale the variables as in [35, 71]. Thus, the dependence on the temperature will appear more explicitly in the energy functional. Let t be the reduced temperature, defined by

$$t := \frac{ac}{b^2},$$

For any $Q \in H^1(\Omega,\, \mathbf{S}_0)$, let Q_* be the function given by

$$Q(x) = \sqrt{\frac{2}{3}}s_*\tilde{Q}_*(x) \qquad \text{for all } x \in \Omega. \tag{1.3.18}$$

We also introduce the constants

$$\eta(t) := \frac{\varepsilon}{\sqrt{a}} = \frac{\varepsilon}{b}\sqrt{\frac{c}{t}}, \qquad h(t) := \frac{\sqrt{24t+1}+1}{144t}. \tag{1.3.19}$$

Of course η depends on ε, b and c as well, but we do not emphasize this dependence as we suppose that the elastic constant is fixed, as well as the material constants b, c.

Lemma 1.3.9. *A function $Q \in H^1(\Omega, \mathbf{S}_0)$ minimizes E_ε in the class $H^1_g(\Omega, \mathbf{S}_0)$ if and only if Q_* minimize*

$$F_t(Q_*) := \int_\Omega \left\{ \frac{1}{2}\left|\nabla Q_*\right|^2 + \frac{1}{\eta^2(t)} f_t(Q_*) \right\} \tag{1.3.20}$$

in the class $H^1_{g_*}(\Omega, \mathbf{S}_0)$, where $g_* := \sqrt{3/2}s_*^{-1}g$ and

$$f_t(Q_*) := \frac{1}{4}\left(1 - |Q_*|^2\right)^2 + h(t)\varphi(Q_*), \qquad \varphi(Q_*) := 1 - 4\sqrt{6}\,\mathrm{tr}\, Q_*^3 + 3|Q_*|^4.$$

Proof. By injecting (1.3.18) into the expression of the energy functional (LG_ε), we obtain

$$E_\varepsilon(Q) = \frac{2s_*^2}{3}\int_\Omega \left\{ \frac{1}{2}\left|\nabla Q_*\right|^2 + \frac{1}{\varepsilon^2} f_*(Q_*) \right\}$$

where

$$f_*(Q_*) := k_0 - \frac{a}{2}\,\mathrm{tr}\, Q_*^2 - \frac{s_* b}{3}\sqrt{\frac{2}{3}}\,\mathrm{tr}\, Q_*^3 + \frac{s_*^2 c}{6}\left(\mathrm{tr}\, Q_*^2\right)^2.$$

The coefficients of f_* can be rewritten in terms of t, and we obtain

$$\begin{aligned}
\frac{s_* b}{3}\sqrt{\frac{2}{3}} &= \frac{b\sqrt{24ac+b^2}+b^2}{6\sqrt{6}c} = 4\sqrt{6}a\,h(t),\\
\frac{s_*^2 c}{6} = \frac{\left(\sqrt{24ac+b^2}+b\right)^2}{96c} &= \frac{b\sqrt{24ac+b^2}+b^2}{48c} + \frac{a}{4} = 3a\,h(t) + \frac{a}{4}.
\end{aligned}$$

Therefore,

$$\frac{f_*(Q_*)}{a} = \left(\frac{k_0}{a} - \frac{1}{4} - h(t)\right) + \frac{1}{4}\left(1 - \mathrm{tr}\, Q_*^2\right)^2 + h(t)\left(1 - 4\sqrt{6}\,\mathrm{tr}\, Q_*^3 + 3\left(\mathrm{tr}\, Q_*^2\right)^2\right)$$

and so

$$E_\varepsilon(Q) = \frac{2s_*^2}{3}\int_\Omega \left\{ \frac{1}{2}\left|\nabla Q_*\right|^2 + \frac{1}{\eta^2(t)} f_t(Q_*) \right\} + C,$$

where $C = C(a,\, b,\, c)$ is some constant. The lemma follows easily. □

The following lemma states an elementary property of the new potential φ.

Lemma 1.3.10. *For all $Q_* \in \mathbf{S}_0$ with $|Q_*| \leq 1$, we have $0 \leq \varphi(Q_*) \leq 8$.*

Proof. From the definition (1.3.9) of $\beta(Q_*)$, we obtain

$$\sqrt{6}\left|\mathrm{tr}\, Q_*^3\right| = \left|Q_*\right|^3 \sqrt{1 - \beta(Q_*)}. \tag{1.3.21}$$

The inequality $\sqrt{1-t} \leq 1 - t/2$, which holds true for $0 \leq t \leq 1$, yields

$$1 - 4\left|Q_*\right|^3 + 3\left|Q_*\right|^4 + 2\beta(Q_*)\left|Q_*\right|^3 \leq \varphi(Q_*) \leq 1 + 4\left|Q_*\right|^3 + 3\left|Q_*\right|^4 - 2\beta(Q_*)\left|Q_*\right|^3.$$

An elementary analysis shows that $1 - 4\left|Q_*\right|^3 + 3\left|Q_*\right|^4 \geq 0$ and $1 + 4\left|Q_*\right|^3 + 3\left|Q_*\right|^4 \leq 8$ when $|Q_*| \leq 1$, whence the lemma follows. □

In view of Lemma 1.3.9, we can restrict our attention to minimizers of the functional F_t, defined by (1.3.20). The vacuum manifold associated with the potential f_t is the set

$$\mathscr{N}_* := \{Q_* \in \mathbf{S}_0\colon f_t(Q_*) = \inf f_t\} = \left\{\sqrt{\frac{3}{2}}\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) : \mathbf{n} \in \mathbb{S}^2\right\}.$$

In particular, after rescaling the variables the vacuum manifold is independent on t. The new manifold coincides with the one we have introduced in Proposition 1.3.3, provided that we take $s_* = \sqrt{3/2}$. In particular, for the manifold $\mathscr{N}_*$

$$\kappa_* = \frac{3}{4}\pi \tag{1.3.22}$$

(this amounts to taking $s_* = \sqrt{3/2}$ in Lemma 1.3.4). Now, consider a t-independent boundary datum $g \in H^1(\partial\Omega,\, \mathscr{N})$, as in Theorem 1.1.1. After change of variable, the corresponding boundary datum for the Q_*-problem is a map $g_* \in H^1(\partial\Omega,\, \mathscr{N}_*)$.

Lemma 1.3.11. *Any minimizer Q_t for the functional F_t in the class $H^1_{g_*}(\Omega,\, \mathbf{S}_0)$ satisfies*

$$Q_t \in C^1(\Omega,\, \mathbf{S}_0) \qquad \textit{and} \qquad \|Q_t\|_{L^\infty(\Omega)} = 1.$$

Proof. The C^1-regularity and the L^∞-upper bound follow by Lemma 1.4.1, by scaling. To show that

$$\|Q_t\|_{L^\infty(\Omega)} \geq 1,$$

note that $|Q|_{|\partial\Omega} = |g_*| = 1$, for g_* takes values in $\mathscr{N}$. □

1.3.3 Proof of Theorem 1.1.1

The following lemma shows that a map which is not maximally biaxial must have an isotropy point. This fact is an easy consequence of the analysis carried out in Subsection 1.3.1. However, it will be crucial in order to obtain a lower estimate for the energy of a non-maximally biaxial configuration.

Lemma 1.3.12. *If $Q \in C^1(\Omega,\, \mathbf{S}_0)$ is* not *maximally biaxial, satisfies $Q_{|\partial\Omega} = g$, and the boundary datum g is non-trivial, then $\min_{\overline{\Omega}} |Q| = 0$.*

Proof. We argue by contradiction, and assume that $s_0 := \sqrt{3/2}\min_{\overline{\Omega}}|Q| > 0$. In view of (1.3.10), the fact that Q is not maximally biaxial implies that $r(Q(x)) \neq 1/2$ for all $x \in \overline{\Omega}$. Since the image of g lies in the vacuum manifold, by a connectedness argument we conclude that $r_0 := \max_{\overline{\Omega}} r(Q) < 1/2$. By (1.3.11), the image of Q is contained in the set

$$\mathscr{N}_0 := \{P \in \mathbf{S}_0\colon s(P) \geq s_0,\, r(P) \leq r_0 < 1/2\}.$$

Now, $\mathscr{N}_0$ is contained in $\mathbf{S}_0 \setminus \mathscr{C}$. In particular, the retraction $\mathscr{R}$ given by Lemma 1.3.6 is well-defined and of class C^1 on $\mathscr{N}_0$. Therefore, $\mathscr{R} \circ Q\colon \omega \to \mathscr{N}$ is a continuous extension of g, which contradicts the non-triviality of g. □

The following proposition is a key step in the proof of Theorem 1.1.1. The proof is adapted from an analogous estimate by Chiron (see [33, Theorem 2]). We introduce following notation. For any $V \subset\subset \mathbb{R}^2$, we define the radius of V as

$$\mathrm{rad}(V) := \inf\left\{\sum_{i=1}^n r_i\colon V \subseteq \bigcup_{i=1}^n B^2(a_i,\, r_i)\right\}. \tag{1.3.23}$$

Proposition 1.3.13. *There exists a constant $M_1 = M_1(\Omega, g)$ and, for each $t > 0$, a number $\varepsilon_0 = \varepsilon_0(t)$ with the following property. If $0 < \varepsilon \leq \varepsilon_0$ and Q_t is a minimizer of* (1.3.20) *satisfying*

$$\min_{\overline{\Omega}} |Q_t| = 0, \tag{1.3.24}$$

then

$$F_t(Q) \geq \kappa_* \log \eta^{-1}(t) - M_1.$$

Proof. For a fixed $\lambda > 0$, we define

$$\Omega_\lambda := \{x \in \Omega\colon\ |Q_\lambda(x)| > \lambda\}, \qquad \omega_\lambda := \{x \in \Omega\colon\ |Q_\lambda(x)| < \lambda\}, \qquad \Gamma_\lambda := \partial\Omega_\lambda \setminus \partial\Omega = \partial\omega_\lambda.$$

The sets Ω_λ, ω_λ, and Γ_λ are non-empty for all $\lambda \in [0, 1]$, due to Lemma 1.3.11. and the assumption (1.3.24). Moreover, Sard lemma implies that Γ_λ is a smooth 1-manifold, for $\mathscr{H}^1$-a.e. λ. We also set

$$\Theta(\lambda) := \int_{\Omega_\lambda} \left|\nabla\left(\frac{Q_\lambda}{|Q_\lambda|}\right)\right|^2, \qquad \nu(\lambda) := \int_{\Gamma_\lambda} |\nabla\, |Q_\lambda||\, \mathrm{d}\mathscr{H}^1.$$

It is well-known that $\nabla Q_t = 0$ a.e. in $\{Q_t = 0\}$, so we can write

$$\int_\Omega |\nabla Q_t|^2 = \int_{\{|Q_t|>0\}} |\nabla Q_t|^2 = \lim_{t\to 0^+} \int_{\Omega_t} |\nabla Q_t|^2$$

by the monotone convergence theorem. This implies

$$\int_\Omega |\nabla Q_t|^2 = \lim_{t\to 0^+} \int_{\Omega_\lambda} \left\{ |\nabla\, |Q_t||^2 + |Q_t|^2 \left|\nabla\left(\frac{Q_t}{|Q_t|}\right)\right|^2 \right\}$$

and, applying the coarea formula, we deduce

$$F_t(Q_t) = \frac{1}{2}\int_0^1 \left\{ \int_{\Gamma_\lambda} \left(|\nabla\, |Q_t|| + \frac{2 f_t(Q_t)}{\eta^2(t)\, |\nabla\, |Q_t||} \right) \mathrm{d}\mathscr{H}^1 - 2\lambda^2 \Theta'(\lambda) \right\} \mathrm{d}\lambda. \tag{1.3.25}$$

Let us estimate the terms in the right-hand side of (1.3.25), starting from the second one. Taking advantage of Lemma 1.3.9 and of Hölder inequality, we obtain

$$\int_{\Gamma_\lambda} \frac{2 f_t(Q_t)}{\eta^2(t)\, |\nabla\, |Q_t||} \geq \frac{(1-\lambda^2)^2}{2\eta^2(t)} \int_{\Gamma_\lambda} \frac{1}{|\nabla\, |Q_t||}\, \mathrm{d}\mathscr{H}^1 \geq \frac{(1-\lambda^2)^2 \mathscr{H}^1(\Gamma_\lambda)^2}{2\eta^2(t)\nu(\lambda)}. \tag{1.3.26}$$

Moreover, we have

$$\mathscr{H}^1(\Gamma_\lambda) \geq 2\,\mathrm{diam}(\Gamma_\lambda) \geq 4\,\mathrm{rad}(\omega_\lambda).$$

Indeed, if $x, y \in \Gamma_\lambda$ are such that $|x - y| = \mathrm{diam}(\Gamma_\lambda)$, then ω_λ is contained in the ball $B^2((x + y)/2, |x-y|/2)$ and hence $\mathrm{rad}(\omega_\lambda) \leq \mathrm{diam}(\Gamma_\lambda)/2$. Combining this fact with (1.3.25) and (1.3.26), we find

$$\begin{aligned} F_t(Q_t) &\geq \frac{1}{2}\int_0^1 \left\{ \nu(\lambda) + \frac{8(1-\lambda^2)^2\, \mathrm{rad}(\omega_\lambda)^2}{\eta^2(t)\nu(\lambda)} \right\} \mathrm{d}\lambda - \int_0^1 \lambda^2 \Theta'(\lambda)\, \mathrm{d}\lambda \\ &\geq \int_0^1 \frac{2\sqrt{2}}{\eta(t)} (1-\lambda^2)\ \mathrm{rad}(\omega_\lambda)\, \mathrm{d}\lambda - \int_0^1 \lambda^2 \Theta'(\lambda)\, \mathrm{d}\lambda. \end{aligned} \tag{1.3.27}$$

The second line follows by the elementary inequality $a + b \geq 2\sqrt{ab}$. As for the last term, we integrate by parts. For all $\lambda_0 > 0$, we have

$$-\int_{\lambda_0}^1 \lambda^2 \Theta'(\lambda)\, \mathrm{d}\lambda = 2\int_{\lambda_0}^1 \lambda\Theta(\lambda)\, \mathrm{d}\lambda + {\lambda_0}^2 \Theta(\lambda_0) \geq 2\int_{\lambda_0}^1 \lambda\Theta(\lambda)\, \mathrm{d}\lambda$$

and, letting $\lambda_0 \to 0$, by monotone convergence ($\Theta \geq 0$, $-\Theta' \geq 0$) we conclude that

$$-\int_0^1 \lambda^2 \Theta'(\lambda)\,\mathrm{d}\lambda \geq 2\int_0^1 \lambda\Theta(\lambda)\,\mathrm{d}\lambda.$$

Arguing as in the proof of Lemmas 1.4.13, 1.4.14, which are based on the results by Sandier (in particular, [123, Theorem 1]), we can establish the bound

$$\Theta(\lambda) \geq -\kappa_* \log\left(\mathrm{rad}(\omega_\lambda)\right) - C \tag{1.3.28}$$

where C depends only on Ω and the boundary datum. In that respect, note that the image of $Q/|Q|$ may lie far from the vacuum manifold. However, the results of Section 1.4 (in particular, Proposition 1.1.2) imply that the set where this occurs is contained in a union of K disks $D_1, \ldots, D_K$, of radius $\lambda_0(h^{-1/2}\eta)(t)$. (Here K, $\lambda_0 > 0$ are independent on ε, t). Moreover, $Q_{t|\Gamma_\lambda}$ defines a non-trivial homotopy class, when ε is small enough. For, if this were not the case, then the Q_t's would converge uniformly in U to a $\mathscr{N}_*$-valued map, due to the results in Sections 1.4 and 1.5. Letting γ is a loop which encircles $D_1, \ldots, D_k$, by Corollary 1.2.2 we have that the homotopy class of $\mathscr{R} \circ Q_{t|\gamma}$ is trivial, so the energy in the region bounded by γ is $\leq C$.

The equations (1.3.27) and (1.3.28) imply

$$F_t(Q_t) \geq \int_0^1 \left\{\frac{2\sqrt{2}}{\eta(t)}\left(1-\lambda^2\right)\mathrm{rad}(\omega_\lambda) - 2\kappa_*\lambda\log\mathrm{rad}(\omega_\lambda)\right\}\mathrm{d}\lambda - C.$$

An easy analysis shows that, when $0 < \lambda < 1$, the function $r \in (0, +\infty) \mapsto 2\sqrt{2}\eta(t)^{-1}(1-\lambda^2)r - 2\kappa_*\lambda\log r$ has a unique minimizer r_*, which is readily computed. As a consequence, we obtain the lower bound

$$\begin{aligned} F_t(Q_t) &\geq \int_0^1 \left\{2\kappa_*\lambda - 2\kappa_*\lambda\log\frac{\eta(t)\kappa_*\lambda}{2\sqrt{2}(1-\lambda^2)}\right\}\mathrm{d}\lambda - C \\ &= -2\kappa_*\int_0^1 \left\{\lambda\log\eta(t) - \lambda + \lambda\log\frac{\kappa_*\lambda}{\sqrt{2}(1-\lambda^2)}\right\}\mathrm{d}\lambda - C. \end{aligned}$$

All the terms are integrable functions of λ on the interval $[0, 1]$, so the proposition follows. ☐

The other key ingredient in the proof of Theorem 1.1.1 is the construction of a biaxial competitor, whose energy is smaller than the lower bound given by Proposition 1.3.13.

Lemma 1.3.14. *Assume that*

$$\eta(t) < R_0 h^{1/2}(t), \tag{1.3.29}$$

where R_0 is a positive constant such that Ω contains a closed disk of radius R_0. Then, there exists a function $P_t \in H^1(\Omega, \mathbf{S}_0)$ such that

$$F_t(P_t) \leq \kappa_*\log\eta^{-1}(t) + \frac{\kappa_*}{2}\log h(t) + M_2,$$

where $M_2 = M_2(\Omega, g)$ is a constant independent on t.

Before giving the proof of the lemma, we show that Lemma 1.3.14 implies Theorem 1.1.1.

Proof of Theorem 1.1.1. Because of (1.3.29), we have

$$\eta(t) \sim \varepsilon t^{-1/2}, \quad h(t) \sim \frac{t^{-1/2}}{12\sqrt{6}} \qquad \text{as } t \to +\infty. \tag{1.3.30}$$

In particular, there exists $t_0 > 0$ such that, for every $t \geq t_0$ there holds

$$-M_1 > \frac{\kappa_*}{2} \log h(t) + M_2. \tag{1.3.31}$$

Fix a value $t \geq t_0$. Thanks to (1.3.30), Condition (1.3.29) is satisfied for ε small enough, depending on t. Let P_t be the function given by Lemma 1.3.14. If the minimizer Q_t satisfies (1.3.24) then, combining (1.3.31) with Lemma 1.3.14 and Proposition 1.3.13, we obtain

$$F_t(P_t) < \kappa_* \log \eta^{-1}(t) - M_1 \leq F_t(Q)\,.$$

This is aa contradiction, so the minimizer cannot satisfy (1.3.24). By Lemma 1.3.11, we have

$$\min_{\overline{\Omega}} |Q_t| > 0.$$

In view of Lemma 1.3.12, we conclude that Q_t is maximally biaxial, that is,

$$\max_{\overline{\Omega}} \beta(Q_t) = 1.$$

Scaling back to Q_ε, and using the fact that β is homogeneous, the theorem follows. □

Proof of Lemma 1.3.14. Let $x_0 \in \Omega$ be such that $D := \overline{B}^2(x_0, R_0) \subseteq \Omega$ (such a point exists, by assumption). Using polar coordinates $(\rho, \theta) \in (0, R_0) \times (0, 2\pi)$, we define the function $P_t \colon D \setminus \{x_0\} \to \mathbf{S}_0$ by

$$P_t\left(x_0 + \rho e^{i\theta}\right) := \sqrt{\frac{3}{2}}\left(r_t^2(\rho) - r_t(\rho) + 1\right)^{-1/2} \left\{\mathbf{n}_0(\theta)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} + r_t(\rho)\left(\mathbf{m}_0(\theta)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right)\right\}, \tag{1.3.32}$$

where $\mathbf{n}_0(\theta) := (\cos\theta/2,\, \sin\theta/2,\, 0)^{\mathsf{T}}$, $\mathbf{m}_0(\theta) := (-\sin(\theta/2),\, \cos(\theta/2),\, 0)^{\mathsf{T}}$ and

$$r_t(\rho) := \begin{cases} 1 - (h^{1/2}\eta^{-1})(t)\rho & \text{if } 0 < \rho \leq (h^{-1/2}\eta)(t) \\ 0 & \text{if } (h^{-1/2}\eta)(t) < \rho \leq R_0. \end{cases} \tag{1.3.33}$$

Notice that $(h^{-1/2}\eta)(t) < R_0$ by (1.3.29), so the function is well-defined. The map P_t can be extended continuously to the point x_0, because

$$\lim_{\rho\to 0^+} P_t(\rho e^{i\theta},\, z) = -\sqrt{\frac{3}{2}}\left(\mathbf{p}_0^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{uniformly on } (\theta,\, z),$$

where $\mathbf{p}_0 := (0,\, 0,\, 1)^{\mathsf{T}}$ (this can be proved by injecting the identity $\mathrm{Id} = \mathbf{n}_0^{\otimes 2} + \mathbf{m}_0^{\otimes 2} + \mathbf{p}_0^{\otimes 2}$ into (1.3.33)). Moreover, $P_{t|\partial D}$ ia a continuous loop $\partial D \to \mathscr{N}_*$, which is not homotopic to a constant. Since g is homotopically non-trivial, we can apply Corollary 1.2.2 and extend P_t to a new function, still denoted P_t, in such a way that $P_t \in H^1(\Omega \setminus D,\, \mathscr{N}_*)$. Then,

$$E_\varepsilon(P_t,\, \Omega \setminus D) = \frac{1}{2}\int_{\Omega\setminus C} |\nabla P_t|^2 \,\mathrm{d}\mathscr{H}^2$$

is a constant, depending only on Ω, C. To conclude, we only need to compute the energy of P_t on the disk D. Note that $|P_t| = 1$ in D, due to (1.3.11). As for the gradient, we have

$$|\nabla P_t|^2 = \left|\frac{\mathrm{d}P_t}{\mathrm{d}\rho}\right|^2 + \frac{1}{\rho^2}\left|\frac{\mathrm{d}P_t}{\mathrm{d}\theta}\right|^2 \begin{cases} \leq C(h^{1/2}\eta^{-1})(t) & \text{where } \rho \leq (h^{-1/2}\eta)(t) \\ = \dfrac{3}{4\rho^2} & \text{where } (h^{-1/2}\eta)(t) \leq \rho \leq 1. \end{cases}$$

Therefore, with the help of Lemma 1.3.10, we obtain

$$\begin{aligned} F_t(P_t) &= \frac{1}{2}\int_D |\nabla P_t|^2 + \frac{h(t)}{\eta^2(t)}\int_D \varphi(P_t) + \frac{1}{2}\int_{\Omega\setminus D} |\nabla P_t|^2 \\ &\leq \pi \int_{(h^{-1/2}\eta)(t)}^{1/2} \frac{3}{4\rho}\,\mathrm{d}\rho + \frac{8h(t)}{\eta^2(t)}\mathscr{H}^2\left(B^2(x_0,\,(h^{-1/2}\eta)(t))\right) + C \\ &\leq \frac{3}{4}\pi \log\left((h^{1/2}\eta^{-1})(t)\right) + C. \end{aligned}$$

Since $\kappa_* = 3/4$ by (1.3.22), the lemma is proved. □

Remark 1.3.3. Since this argument does not provide an explicit lower bound for $|Q_t|$, we cannot infer that singularity profiles (as defined in Section 1.1) are bounded away from zero. A more detailed discussion of the profile of two-dimensional minimizers can be found in [41].

1.4 Asymptotic analysis of the minimizers

This section investigates the behaviour of minimizers of (P_ε) as $\varepsilon \searrow 0$, and contains the proofs of Proposition 1.1.2 and Theorem 1.1.3. We start by recalling some well-known properties of minimizers.

Lemma 1.4.1. *Any minimizer u_ε of (P_ε) is of class C^1 up to the boundary of Ω, and satisfies*

$$\|u_\varepsilon\|_{L^\infty(\Omega)} \leq 1, \qquad \|\nabla u_\varepsilon\|_{L^\infty(\Omega)} \leq \frac{C}{\varepsilon}.$$

Proof. Minimizers solve the Euler-Lagrange equation (1.2.1) associated with E_ε, whence the C^1-regularity follows by classical elliptic theory (once the L^∞-bound is proved). The L^∞-bound on u_ε can be easily established via a comparison argument. Assume, by contradiction, that $|u_\varepsilon(x_0)| > 1$ for some $x_0 \in \Omega$, and define

$$v_\varepsilon(x) := \begin{cases} u_\varepsilon(x) & \text{if } |u_\varepsilon(x)| \leq 1 \\ \dfrac{u_\varepsilon(x)}{|u_\varepsilon(x)|} & \text{otherwise.} \end{cases}$$

Clearly $|\nabla v_\varepsilon| \leq |\nabla u_\varepsilon|$ and, by (H_3), $f(v_\varepsilon) \leq f(u_\varepsilon)$, with strict equality at least at the point x_0. Thus, $E_\varepsilon(v_\varepsilon) < E_\varepsilon(u_\varepsilon)$, which contradicts the minimality of u_ε. Once the LL^∞-bound for u_ε is prove, the bound on the gradient follows by Equation (1.2.1), with the help of [13, Lemma A.2]. □

Lemma 1.4.2 (Pohozaev identity)**.** *Let $G \subseteq \mathbb{R}^2$ be any subdomain of Ω, and $x_0 \in G$. Denote by ν the unit outward-pointing normal to ∂G and by τ the unit tangent to ∂G, oriented so that $(\tau,\,\nu)$ is direct. Then, any solution u_ε of Equation* (1.2.1) *satisfies*

$$\begin{aligned} &\frac{1}{\varepsilon^2}\int_G f(u_\varepsilon) + \frac{1}{2}\int_{\partial G} (x - x_0)\cdot\nu \left|\frac{\partial u_\varepsilon}{\partial \nu}\right|^2 \mathrm{d}\mathscr{H}^1 \\ &\qquad = \int_{\partial G} \left\{ \frac{1}{2}(x - x_0)\cdot\nu \left|\frac{\partial u_\varepsilon}{\partial \tau}\right|^2 - (x - x_0)\cdot\tau \frac{\partial u_\varepsilon}{\partial \nu} : \frac{\partial u_\varepsilon}{\partial \tau} + (x - x_0)\cdot\nu \frac{1}{\varepsilon^2} f(u_\varepsilon) \right\} \mathrm{d}\mathscr{H}^1. \end{aligned}$$

Proof. The lemma can be proved arguing exactly as in [14, Theorem III.2]. For the sake of completeness, we give here the proof, assuming that $G \subseteq \mathbb{R}^n$ for any $n \geq 2$ (the case $n = 3$ will be useful in Chapter 2). Up to a translation, we may assume $x_0 = 0$. We drop out the subscript ε, for the sake of convenience. We multiply both sides of Equation (1.2.1) by $x_k \partial_k u_{ij,k}$ (where $u_{ij,k} := \partial_{x_k} u_{ij}$), sum over i, j, k and integrate over G:

$$-\int_G u_{ij,hh}\, x_k u_{ij,k} + \frac{1}{\varepsilon^2}\int_G \frac{\partial f(u)}{\partial u_{ij}}\, u_{ij,k}\, x_k = 0. \tag{1.4.1}$$

We integrate by parts the first term:

$$-\int_G u_{ij,hh}\, x_k u_{ij,k} = \int_G u_{ij,h}\left(\delta_{kh} u_{ij,k} + x_k u_{ij,kh}\right) - \int_{\partial G} u_{ij,h}\nu_h\, u_{ij,k} x_k \,\mathrm{d}\mathscr{H}^{n-1}.$$

Since

$$\int_G x_k\, u_{ij,h} u_{ij,kh} = \frac{1}{2}\int_G x_k\,\partial_k\big(u_{ij,h}u_{ij,h}\big) = \\ -\frac{n}{2}\int_G u_{ij,h}u_{ij,h} + \frac{1}{2}\int_{\partial G} u_{ij,h}u_{ij,h}\, x_k\nu_k \,\mathrm{d}\mathscr{H}^{n-1},$$

we get

$$(1.4.2)\qquad -\int_G u_{ij,\,hh}\, x_k u_{ij,\,k} = \left(1 - \frac{n}{2}\right)\int_G u_{ij,h}u_{ij,h} \\ - \int_{\partial G} u_{ij,\,h}\nu_l\, u_{ij,\,k} x_k \,\mathrm{d}\mathscr{H}^{n-1} + \frac{1}{2}\int_{\partial G} u_{ij,\,h}u_{ij,\,h}\, x_k\nu_k \,\mathrm{d}\mathscr{H}^{n-1}.$$

Now, we integrate by parts the second term in (1.4.1):

$$(1.4.3)\qquad \frac{1}{\varepsilon^2}\int_G \partial_k\big(f(u_\varepsilon)\big)\, x_k = -\frac{1}{\varepsilon^2}\int_G f(u_\varepsilon) + \frac{1}{\varepsilon^2}\int_{\partial G} f(u_\varepsilon) x_k\nu_k \,\mathrm{d}\mathscr{H}^{n-1}.$$

Combining (1.4.1), (1.4.2) and (1.4.3) we obtain

$$(1.4.4)\qquad \int_{\partial G} (x\cdot\nu)\left\{\frac{1}{2}\left|\nabla u_\varepsilon\right|^2 + \frac{1}{\varepsilon^2} f(u_\varepsilon)\right\}\mathrm{d}\mathscr{H}^{n-1} \\ = \int_{\partial G} \big(\nabla u_\varepsilon\cdot x\big)\big(\nabla u_\varepsilon\cdot\nu\big)\,\mathrm{d}\mathscr{H}^{n-1} + \int_G \left\{\left(\frac{n}{2} - 1\right)\left|\nabla u_\varepsilon\right|^2 + \frac{1}{\varepsilon^2} f(u_\varepsilon)\right\}.$$

Finally, when $n = 2$, we conclude the proof of the lemma with the help of the identities

$$\big(\nabla u_\varepsilon\cdot x\big)\big(\nabla u_\varepsilon\cdot\nu\big) = (x\cdot\nu)\left|\frac{\partial u_\varepsilon}{\partial\nu}\right|^2 + (x\cdot\tau)\frac{\partial u_\varepsilon}{\partial\nu}\cdot\frac{\partial u_\varepsilon}{\partial\tau}, \qquad \left|\nabla u_\varepsilon\right|^2 = \left|\frac{\partial u_\varepsilon}{\partial\nu}\right|^2 + \left|\frac{\partial u_\varepsilon}{\partial\tau}\right|^2. \qquad \square$$

Remark 1.4.1. When considering the Landau-de Gennes equation (1.2.3), the additional Id-term does not play any role in the proof of the Pohozaev identity. Indeed, assume $x_0 = 0$, multiply both sides of (1.2.3) by $x_k Q_{ij,\,k}$, sum over i, j, k and integrate over G. We obtain

$$-\int_G Q_{\varepsilon,\,ij,\,ll}\, x_k Q_{\varepsilon,\,ij,\,k}\,\mathrm{d}x + \frac{1}{2\varepsilon^2}\int_G \frac{\partial f(Q_\varepsilon)}{\partial Q_{\varepsilon,\,ij}}\, Q_{\varepsilon,\,ij,\,k}\, x_k\,\mathrm{d}x + \frac{1}{3} b\int_G x_k Q_{\varepsilon,\,ii,\,k}\,\mathrm{tr}\, Q_\varepsilon^2\,\mathrm{d}x = 0,$$

and the third integral vanishes, since $Q_{\varepsilon,\,ii} = 0$. The proof follows exactly as in the previous case; the reader is referred to [98, Lemma 2] for more details.

Lemma 1.4.3. *Let $\Omega \subseteq \mathbb{R}^2$ and let u_ε be a minimizer for Problem* (P_ε)*. Then, there exists a constant C, depending on Ω and G, such that*

$$E_\varepsilon(u_\varepsilon) \leq \kappa_*\left|\log\varepsilon\right| + C.$$

Proof. The proof of this lemma is a slightly different version of [14, Theorem III.1] (see also [33]). Let $(\eta_1,\,\eta_2,\,\ldots,\,\eta_m) \in \Gamma(\mathscr{N})^m$ be an m-uple which achieve the minimum in (1.2.9), that is,

$$(1.4.5)\qquad \prod_{j=1}^{m}\eta_j \cap \prod_{i=1}^{k}\gamma_i \neq \emptyset, \qquad \frac{1}{4\pi}\sum_{j=1}^{m}\lambda^2(\eta_j) = \kappa_*,$$

and for each $j \in \{1,\,\ldots,\,m\}$ choose a loop $b_j \in \eta_j$, of minimal length (i.e., $\lambda(\eta_j) = 2\pi|b_j'|$). Let $B_1,\,\ldots,\,B_m$ be mutually disjoint, closed disks in Ω, of radius r. Applying Lemma 1.2.1, we find a smooth function $v\colon \Omega\setminus\cup_{j=1}^m B_j \to \mathscr{N}$, such that $v = g$ on $\partial\Omega$ and $v = b_j$ on ∂B_j, for each j.

We extend v to a function $v_\varepsilon\colon \overline{\Omega} \to \mathscr{N}$ in the following way. On $\Omega \setminus \cup_{j=1}^m B_j$, set $v = v_\varepsilon$, whereas on each ball B_j, denoting by $(\rho,\, \theta)$ the polar coordinates around the center x_j of the ball, set

$$v_\varepsilon(x) := \begin{cases} \varepsilon^{-1}\rho\, b_j\left(x_j + re^{i\theta}\right) & \text{if } 0 < \rho < \varepsilon \\ b_j\left(x_j + re^{i\theta}\right) & \text{if } \varepsilon \leq \rho < r. \end{cases}$$

Since $v_\varepsilon \in H^1_g(\Omega,\, \mathbb{R}^k)$, the minimality of u_ε entails $E_\varepsilon(u_\varepsilon) \leq E_\varepsilon(v_\varepsilon)$. Now, we compute $E_\varepsilon(v_\varepsilon)$:

$$E_\varepsilon(v_\varepsilon,\, \Omega \setminus \bigcup_{j=1}^m B_j) = \frac{1}{2}\int_{\Omega\setminus\bigcup_{j=1}^m B_j} |\nabla v|^2 = C,$$
$$E_\varepsilon(v_\varepsilon,\, B_j) \leq \int_{B_j} C\varepsilon^{-2} \leq C,$$

and, passing to polar coordinates,

$$E_\varepsilon(v_\varepsilon,\, B_j \setminus B_\varepsilon(x_j)) = \frac{1}{2}\int_\varepsilon^r \frac{\mathrm{d}\rho}{\rho}\int_{\mathbb{S}^1} d\omega\, \left|b_j'(\omega)\right|^2 \leq \frac{1}{4\pi}\lambda^2(\eta_j)\left|\log\varepsilon\right| + C.$$

Combining these bounds, with the help of (1.4.5) we conclude. □

1.4.1 Localizing the singularities

In this subsection, we will prove Proposition 1.1.2. Namely, we will show that the image of u_ε lies close to the vacuum manifold, except on the union of a finite number of small balls. Analogous results have been established for the Ginzburg-Landau model in [14], in case the domain $\Omega \subseteq \mathbb{R}^2$ is star-shaped. The star-shapedness assumption can been removed, by using a local version of the arguments of [14]. This technique has been introduced independently by Struwe [136] and Bethuel and Rivière [18] (see also [12] for more details). We introduce a (small) parameter $0 < \alpha \leq 1$, whose value is going to be adjusted later, and we set

$$e_\varepsilon(u_\varepsilon) := \frac{1}{2}\left|\nabla u_\varepsilon\right|^2 + \frac{1}{\varepsilon^2} f(u_\varepsilon).$$

We claim the following

Proposition 1.4.4. *Let $\alpha \in (0,\, 1]$, $\delta \in (0,\, \delta_0)$ be fixed. There exists ε_0 and, for any $0 < \varepsilon \leq \varepsilon_0$, a finite set $X_\varepsilon = \{x_1^\varepsilon,\, \ldots,\, x_{k_\varepsilon}^\varepsilon\} \subseteq \Omega$, whose cardinality is bounded independently of ε, such that*

$$\operatorname{dist}(u_\varepsilon(x),\, \mathscr{N}) \leq \delta \qquad \text{if } \operatorname{dist}(x,\, X_\varepsilon) > \lambda_0\varepsilon, \tag{1.4.6}$$

where $\lambda_0 > 0$ is a constant independent of ε, and

$$\varepsilon^{4\alpha} e_\varepsilon(u_\varepsilon)(x) \leq C_\alpha \qquad \text{if } \operatorname{dist}(x,\, X_\varepsilon) > \varepsilon^\alpha. \tag{1.4.7}$$

Proposition 1.4.4 clearly implies Proposition 1.1.2. As a first step in the proof, we show that $e_\varepsilon(u_\varepsilon)$ solves an elliptic inequality, in the regions where u_ε lies close to the vacuum manifold.

Lemma 1.4.5. *Assume $\omega \subseteq \Omega$ is an open set, such that $\operatorname{dist}(u_\varepsilon(x),\, \mathscr{N}) \leq \delta$ holds for all $x \in \omega$ and all $\varepsilon > 0$. Then, $e_\varepsilon(u_\varepsilon)$ solves pointwise in ω the inequality*

$$-\Delta e_\varepsilon(u_\varepsilon) \leq C e_\varepsilon^2(u_\varepsilon).$$

Proof. Reminding that u_ε is a solution of Equation (1.2.1), we compute plainly

$$-\frac{1}{2}\Delta\left|\nabla u_\varepsilon\right|^2 = -\nabla\left(\Delta u_\varepsilon\right)\cdot\nabla u_\varepsilon - \left|\nabla^2 u_\varepsilon\right|^2 = -\frac{1}{\varepsilon^2}\nabla u_\varepsilon : \mathrm{D}^2 f(u_\varepsilon)\nabla u_\varepsilon - \left|\nabla^2 u_\varepsilon\right|^2,$$

where $\left|\nabla^2 u_\varepsilon\right|^2 = \sum_{i,j} |\partial_i \partial_j u_\varepsilon|^2$, and

$$\begin{aligned} -\frac{1}{\varepsilon^2}\Delta f(u_\varepsilon) &= -\frac{1}{\varepsilon^2}\nabla\left(\mathrm{D}f(u_\varepsilon)\right)\cdot\nabla u_\varepsilon - \frac{1}{\varepsilon^2}\mathrm{D}f(u_\varepsilon) : \Delta u_\varepsilon \\ &= -\frac{1}{\varepsilon^2}\nabla u_\varepsilon : \mathrm{D}^2 f(u_\varepsilon)\nabla u_\varepsilon - \frac{1}{\varepsilon^4}\left|\mathrm{D}f(u_\varepsilon)\right|^2. \end{aligned}$$

Adding these contributions, we obtain

$$-\Delta e_\varepsilon(u_\varepsilon) + \left|\nabla^2 u_\varepsilon\right|^2 + \frac{1}{\varepsilon^4}\left|\mathrm{D}f(u_\varepsilon)\right|^2 = -\frac{2}{\varepsilon^2}\nabla u_\varepsilon \cdot \mathrm{D}^2 f(u_\varepsilon)\nabla u_\varepsilon. \tag{1.4.8}$$

Hypothesis (H_2) provides

$$\frac{1}{\varepsilon^4}\left|\mathrm{D}f(u_\varepsilon)\right|^2 \geq \frac{m_0}{\varepsilon^4}\,\mathrm{dist}^2(u_\varepsilon,\,\mathscr{N}). \tag{1.4.9}$$

Moreover, the image $u_\varepsilon(\omega)$ lies close to $\mathscr{N}$ by assumption, so the right-hand side of (1.4.8) can be estimated by the local Lipschitz continuity of $\mathrm{D}^2 f$:

$$\begin{aligned} -\frac{2}{\varepsilon^2}\nabla u_\varepsilon : \mathrm{D}^2 f(u_\varepsilon)\nabla u_\varepsilon &\leq -\frac{2}{\varepsilon^2}\nabla u_\varepsilon : \mathrm{D}^2 f(\pi(u_\varepsilon))\nabla u_\varepsilon + \frac{2}{\varepsilon^2}\left|\mathrm{D}^2 f(u_\varepsilon) - \mathrm{D}^2 f(\pi(u_\varepsilon))\right|\left|\nabla u_\varepsilon\right|^2 \\ &\leq -\frac{2}{\varepsilon^2}\nabla u_\varepsilon : \mathrm{D}^2 f(\pi(u_\varepsilon))\nabla u_\varepsilon + \frac{C}{\varepsilon^2}\,\mathrm{dist}(u_\varepsilon,\,\mathscr{N})\left|\nabla u_\varepsilon\right|^2 \\ &\leq \frac{C}{\varepsilon^2}\,\mathrm{dist}(u_\varepsilon,\,\mathscr{N})\left|\nabla u_\varepsilon\right|^2. \end{aligned}$$

For the latter inequality, remind that every point $\mathbf{p} \in \mathscr{N}$ is a minimizer for f, so $\mathrm{D}^2 f(\mathbf{p}) \geq 0$. We infer

$$-\frac{2}{\varepsilon^2}\nabla u_\varepsilon : \mathrm{D}^2 f(u_\varepsilon)\nabla u_\varepsilon \leq \frac{m_0}{\varepsilon^4}\,\mathrm{dist}^2(u_\varepsilon,\,\mathscr{N}) + C\left|\nabla u_\varepsilon\right|^4$$

and the first term can be reabsorbed in the left-hand side of (1.4.8), by means of (1.4.9). This concludes the proof. □

Our next ingredient is a Clearing Out lemma, which relies crucially on (H_2).

Proposition 1.4.6 (Clearing Out)**.** *There exist some positive constants λ_0 and μ_0 with the following property: for all $x_0 \in \Omega$ and all $l \in [\lambda_0\varepsilon,\, 1]$, if the minimizer u_ε satisfies*

$$\frac{1}{\varepsilon^2}\int_{B(x_0,\,2l)\cap\Omega} f(u_\varepsilon) \leq \mu_0 \tag{1.4.10}$$

then

$$\mathrm{dist}(u_\varepsilon(x),\,\mathscr{N}) \leq \delta \qquad \textit{for all } x \in B(x_0,\,l)\cap\Omega. \tag{1.4.11}$$

Proof. Set

$$f_0 := \min\left\{f(v)\colon\ \mathrm{dist}(v,\,\mathscr{N}) \geq \delta,\ |v| \leq 1\right\},$$

and remark that $f_0 > 0$, because it is the minimum of a strictly positive function on a compact set. We define

$$\lambda_0 := \frac{\delta}{2C}, \qquad \mu_0 := \frac{\pi}{2}\lambda_0^2\,\min\left\{f_0,\ \frac{1}{8}m_0\delta^2\right\}, \tag{1.4.12}$$

where C is a constant such that $|\nabla u_\varepsilon| \leq C\varepsilon^{-1}$ (such a constant exists, by Lemma 1.4.1). We are going to check that this choice of λ_0, μ_0 works. To do so, we proceed by contradiction and assume there is some point $x \in B(x_0, l)$ such that $\mathrm{dist}(u_\varepsilon(x), \mathscr{N}) > \delta$. Firstly, we remark that this assumption implies $\mathrm{dist}(x, \partial\Omega) > \lambda_0\varepsilon$. Indeed, if it were $\mathrm{dist}(x, \partial\Omega) \leq \lambda_0\varepsilon$ then, in view of (H_4), we would have

$$\mathrm{dist}(u_\varepsilon(x), \mathscr{N}) \leq \|\nabla u_\varepsilon\|_{L^\infty} \mathrm{dist}(x, \partial\Omega) \leq C\lambda_0 = \frac{\delta}{2}.$$

It follows that the ball $B(x, \lambda_0\varepsilon)$ is entirely contained in $B(x_0, 2l) \cap \Omega$. In addition, for all $y \in B(x, \lambda_0\varepsilon)$ we have

$$\mathrm{dist}(u_\varepsilon(y), \mathscr{N}) \geq \mathrm{dist}(u_\varepsilon(x), \mathscr{N}) - |u_\varepsilon(x) - u_\varepsilon(y)| > \delta - \lambda_0\varepsilon \|\nabla u_\varepsilon\|_{L^\infty} \geq \frac{\delta}{2}.$$

Due to Remark 1.2.4 and Lemma 1.4.1, this implies

$$\frac{1}{\varepsilon^2}\int_{B(x_0, 2l)\cap\Omega} f(u_\varepsilon) \geq \frac{1}{\varepsilon^2}\int_{B(x, \lambda_0\varepsilon)} f(u_\varepsilon) \geq \pi\lambda_0^2 \min\left\{f_0, \frac{1}{8}m_0\delta^2\right\} = 2\mu_0,$$

which contradicts the assumption (1.4.10). □

The following results can be found in [12, Section IV.5]. For the sake of completeness, we give here a proof.

Lemma 1.4.7. *Set $K_\varepsilon := |\log\varepsilon|^{-1}E_\varepsilon(u_\varepsilon, B(x_0, \varepsilon^\alpha) \cap \Omega)$. For any $x_0 \in \Omega$ and $\varepsilon > 0$, there exists a radius $r = r(x_0, \varepsilon) \in (\varepsilon^\alpha, \varepsilon^{\alpha/2})$ such that*

$$\int_{\partial B(x_0, r)\cap\Omega} \left\{\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon^2}f(u_\varepsilon)\right\} \mathrm{d}\mathscr{H}^1 \leq \frac{2K_\varepsilon}{\alpha r}.$$

Proof. The proof relies on a simple average argument. Assume that the lemma were false. Then, by integrating with respect to $r \in (\varepsilon^{2\alpha}, \varepsilon^\alpha)$, we would obtain

$$E_\varepsilon(u_\varepsilon, B(x_0, \varepsilon^\alpha) \cap \Omega) \geq \frac{2K_\varepsilon}{\alpha}\int_{\varepsilon^{2\alpha}}^{\varepsilon^\alpha} \frac{\mathrm{d}r}{r} = 2K_\varepsilon |\log\varepsilon| = 2E_\varepsilon(u_\varepsilon, B(x_0, \varepsilon^\alpha) \cap \Omega),$$

which implies $E_\varepsilon(u_\varepsilon, B(x_0, \varepsilon^\alpha) \cap \Omega) = 0$. Therefore, on the set $B(x_0, r) \cap \Omega$ we have $u_\varepsilon = u_*$, where $u_* \in \mathscr{N}$ is a constant. In particular, the lemma is satisfied. This is a contradiction, and yields the conclusion of the proof. □

Lemma 1.4.8. *Let $x_0 \in \Omega$. There exists a constant C_α, depending only on α, g and Ω, such that*

$$\frac{1}{\varepsilon^2}\int_{B(x_0, \varepsilon^\alpha)\cap\Omega} f(u_\varepsilon) \leq C_\alpha.$$

Proof. Combining Lemma 1.4.7 with the upper bound on the energy given by 1.4.3, for any ε small enough we find a radius $r = r(x_0, \varepsilon) \in (\varepsilon^{2\alpha}, \varepsilon^\alpha)$ such that

$$\int_{\partial B(x_0, r)\cap\Omega} \left\{\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon^2}f(u_\varepsilon)\right\} \mathrm{d}\mathscr{H}^1 \leq \frac{4\kappa_*}{\alpha r}. \tag{1.4.13}$$

Of course, assuming that ε is small yields no loss of generality in the proof of the lemma. Assume for the moment that $B(x_0, r) \subseteq \Omega$. Then, by applying the Pohozaev inequality (Lemma 1.4.2) with $G = B(x_0, r)$, we obtain

$$\frac{1}{\varepsilon^2}\int_{B(x_0, r)} f(u_\varepsilon) \leq r\int_{\partial B(x_0, r)} \left\{\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon^2}f(u_\varepsilon)\right\} \mathrm{d}\mathscr{H}^1 \overset{(1.4.13)}{\leq} \frac{4\kappa_*}{\alpha}$$

which proves the lemma, in this case. It remains to consider the case $B(x_0, r) \not\subseteq \Omega$. Set $\Gamma := B(x_0, r) \cap \partial\Omega \neq \emptyset$, so that

$$\partial\left(B(x_0, r) \cap \Omega\right) = \left(\partial B(x_0, r) \cap \Omega\right) \cup \Gamma.$$

Pick some $x_1 \in \Omega$. By applying Lemma 1.4.2 and (1.4.13) again, with $G = B(x_0, r) \cap \Omega$ and x_1 instead of x_0, we deduce

$$\begin{aligned}\frac{1}{\varepsilon^2}\int_{B(x_0,\, r)\cap\Omega} f(u_\varepsilon) &+ \frac{1}{2}\int_\Gamma (x - x_1)\cdot\nu \left|\frac{\partial u_\varepsilon}{\partial \nu}\right|^2 \mathrm{d}\mathscr{H}^1 \\ &\leq C_\alpha + \frac{1}{2}\int_\Gamma (x - x_1)\cdot\nu \left|\frac{\partial g}{\partial \tau}\right|^2 \mathrm{d}\mathscr{H}^1 - \int_\Gamma (x - x_1)\cdot\tau \frac{\partial u_\varepsilon}{\partial\nu}\cdot\frac{\partial g}{\partial\tau}\,\mathrm{d}\mathscr{H}^1\end{aligned}$$

(recall that $f(g) = 0$, by (H_4)). Here ν is the outward normal to $\partial\Omega$ and τ is a unit tangent vector to $\partial\Omega$, oriented so that (τ, ν) is a direct couple. Then, by applying the elementary inequality $ab \leq a^2 + b^2/4$, we obtain

$$\frac{1}{\varepsilon^2}\int_{B(x_0,\, r)\cap\Omega} f(u_\varepsilon) + \frac{1}{2}\int_\Gamma (x - x_1)\cdot\nu \left|\frac{\partial u_\varepsilon}{\partial \nu}\right|^2 \mathrm{d}\mathscr{H}^1 \leq C_\alpha + \frac{1}{4}\int_\Gamma \left|(x - x_1)\cdot\tau\right| \left|\frac{\partial u_\varepsilon}{\partial \nu}\right|^2 \mathrm{d}\mathscr{H}^1. \tag{1.4.14}$$

Let $\sigma(x_0)$ be the nearest-point projection of x_1 on $\partial\Omega$. We choose

$$x_1 := \sigma(x_0) - 4r\,\nu(\sigma(x_0)),$$

which belongs to Ω if ε (and hence r) is small enough. When ε is small we also have

$$(x - x_1)\cdot\nu \geq 0, \qquad \frac{1}{2}\left|(x - x_1)\cdot\tau\right| \leq (x - x_1)\cdot\nu \qquad \text{on } \Gamma,$$

thus the lemma follows by (1.4.14). □

Proposition 1.4.9. *There exist positive constants ε_0 and η_α, independent of ε, with the following property: if $0 < \varepsilon \leq \varepsilon_0$ and a point $x_0 \in \Omega$ satisfies*

$$\int_{B(x_0,\, 2\varepsilon^{\alpha/2})\cap\Omega} |\nabla u_\varepsilon|^2 \leq \eta_\alpha \left|\log\varepsilon\right| + C \tag{1.4.15}$$

then $\mathrm{dist}(u_\varepsilon(x),\, \mathscr{N}) \leq \delta$ *for all* $x \in B(x_0,\, \varepsilon^\alpha) \cap \Omega$.

Proposition 1.4.9 provides a concentration result for the energy, which will be crucial in our argument.

Proof of Proposition 1.4.9. Due to the assumption (1.4.15) and the average argument of Lemma 1.4.7, there exists $r = r(x_0,\, \varepsilon) \in (2\varepsilon^\alpha,\, 2\varepsilon^{\alpha/2})$ such that

$$\int_{\partial B(x_0,\, r)\cap\Omega} \left\{\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon^2} f(u_\varepsilon)\right\} \mathrm{d}\mathscr{H}^1 \leq \frac{4}{\alpha r}\left(\eta_\alpha + C\left|\log\varepsilon\right|^{-1}\right).$$

In particular, if $\varepsilon \leq \varepsilon_0$ for some small ε_0, we have

$$\int_{\partial B(x_0,\, r)\cap\Omega} \left\{\frac{1}{2}|\nabla u_\varepsilon|^2 + \frac{1}{\varepsilon^2} f(u_\varepsilon)\right\} \mathrm{d}\mathscr{H}^1 \leq \frac{8\eta_\alpha}{\alpha r}.$$

Arguing as in the proof of Lemma 1.4.8, we deduce

$$\frac{1}{\varepsilon^2}\int_{B(x_0,\, r)\cap\Omega} f(u_\varepsilon) \leq \frac{C\eta_\alpha}{\alpha} + C\varepsilon_0^\alpha \tag{1.4.16}$$

for some $(\alpha,\, \varepsilon)$-independent constant C. (The contribution coming from the integrals on $B(x_0,\, r) \cap \partial\Omega$, if any, is bounded by $C\varepsilon^\alpha$.) Now, choose η_α and ε_0 so small that

$$\frac{C\eta_\alpha}{\alpha} + C\varepsilon_0^\alpha < \mu_0 \qquad \text{and} \qquad \lambda_0\varepsilon_0 \leq \varepsilon_0^{2\alpha}$$

where μ_0, λ_0 are the constants given by Proposition 1.4.6. Then, Proposition 1.4.6 (with $l = \varepsilon^\alpha$) and (1.4.16) imply that $\mathrm{dist}(u_\varepsilon(x),\, \mathscr{N}) \leq \delta$ for any $x \in B(x_0,\, \varepsilon^\alpha) \cap \Omega$). □

Reducing, if necessary, the value of η_α, we are able to show another estimate for minimizers satisfying (1.4.15). This will be the final ingredient in our proof of Proposition 1.4.4.

Proposition 1.4.10. *There exist constants η_α, $C_\alpha > 0$ (with C_α depending only on α, η_α) such that, if u_ε satisfies the condition (1.4.15) for some $x_0 \in \Omega$, then*

$$\varepsilon^{4\alpha} e_\varepsilon(u_\varepsilon)(x_0) \leq C_\alpha.$$

Proof. We suppose, at first, that $B(x_0,\, \varepsilon^\alpha) \subseteq \Omega$. In view of Proposition 1.4.9, we can assume that $\operatorname{dist}(u_\varepsilon,\, \mathscr{N}) \leq \delta$ on $B(x_0,\, \varepsilon^\alpha)$. Furthermore, (1.4.15) and Lemma 1.4.8 provide

$$E_\varepsilon(u_\varepsilon,\, B(x_0,\, \varepsilon^\alpha) \cap \Omega) \leq \eta_\alpha \left|\log \varepsilon\right| + C_\alpha. \tag{1.4.17}$$

Using (1.4.17) and Lemma 1.4.7, for ε small enough we find $r \in (\varepsilon^{2\alpha},\, \varepsilon^\alpha)$ such that

$$\int_{\partial B(x_0,\, r)\cap\Omega} \left\{ \frac{1}{2} \left|\nabla u_\varepsilon\right|^2 + \frac{1}{\varepsilon^2} f(u_\varepsilon) \right\} \mathrm{d}\mathscr{H}^1 \leq \frac{4\eta_\alpha}{\alpha r}. \tag{1.4.18}$$

Now, set

$$\epsilon := \varepsilon / r \qquad \text{and} \qquad v_\epsilon(x) := u_\varepsilon\left(\frac{x}{r} + x_0\right) \qquad \text{for } x \in B := B(0,\, 1).$$

As a consequence of the scaling, we deduce $e_\epsilon(v_\epsilon) = r^2 e_\varepsilon(u_\varepsilon)$, hence

$$E_\epsilon(v_\epsilon,\, B) = E_\varepsilon(u_\varepsilon,\, B(x_0,\, r))$$

and v_ϵ minimizes the energy E_ϵ among the maps $w \in H^1(B,\, \mathbb{R}^d)$, with $w_{|\partial B} = v_{\epsilon|\partial B}$. Moreover, (1.4.18) transforms into

$$\int_{\partial B} e_\epsilon(v_\epsilon)\, \mathrm{d}\mathscr{H}^1 \leq \frac{4\eta_\alpha}{\alpha}. \tag{1.4.19}$$

We will take advantage of the following property, whose proof is postponed.

Lemma 1.4.11. *The energy of v_ϵ is controlled by η_α, that is,*

$$\int_B e_\epsilon(v_\epsilon) \leq C_\alpha \eta_\alpha.$$

Recall also that, due to Lemma 1.4.5, $e_\epsilon(v_\epsilon)$ solves an elliptic inequality. Thus, we are in position to invoke a result by Chen and Struwe ([32] — the reader is also referred to [127, Theorem 2.2]): provided that η_α is small enough, Lemma 1.4.11 implies the estimate

$$r^2 e_\varepsilon(u_\varepsilon)(x_0) = e_\epsilon(v_\epsilon)(x) \leq \int_B e_\epsilon(v_\epsilon) \leq C_\alpha \eta_\alpha.$$

This concludes the proof, in case $B(x_0,\, \varepsilon^\alpha)$ does not intersect the boundary.

We still have to cover the case $B(x_0,\, \varepsilon^\alpha) \nsubseteq \Omega$, but this entail no significant change in the proof (nor in the proof of Lemma 1.4.11). As we deal with a local result, we can straighten the boundary and assume that Ω coincides locally with the set $\mathbb{R}^n_+$. In place of the Chen-Struwe result we can exploit [127, Theorem 2.6], which deals with the Dirichlet boundary condition. $\square$

Proof of Lemma 1.4.11. We split the proof in steps, for clarity.

Step 1 (Construction of the harmonic extension). The composition $\pi(v_\epsilon)$ is well defined, since the image of v_ϵ lies close to the vacuum manifold. Set $\sigma_\epsilon := \operatorname{dist}(v_\epsilon,\, \mathscr{N}) = |v_\epsilon - \pi(v_\epsilon)|$, and denote by ω_ϵ an harmonic extension of $\pi(v_\epsilon)_{|\partial B}$ on B. The existence of such an extension is a classical result by Morrey (see, for instance, [105]). Lemma 4.2 in [125] and (1.4.11) imply that

$$\int_B |\nabla\omega_\epsilon|^2 \leq C \int_{\partial B} e_\epsilon(v_\epsilon)\,\mathrm{d}\mathscr{H}^1 \leq C_\alpha \eta_\alpha. \tag{1.4.20}$$

We wish to use ω_ϵ as a comparison map, in order to obtain the H^1 bound for v_ϵ. To do so, we have to take care of the boundary condition on ∂D.

Step 2 (An auxiliary map). It will be useful to introduce an auxiliary map φ_ϵ. Using polar coordinates on D, we define φ_ϵ by the formula

$$\varphi_\epsilon(\rho,\,\theta) = \begin{cases} \epsilon^{-1}(\rho - 1 + \epsilon)\sigma_\epsilon(\theta) & \text{if } 1-\epsilon \leq \rho \leq 1 \\ 0 & \text{if } \rho < 1 - \epsilon, \end{cases}$$

We claim that

$$\int_B \left\{ |\nabla\varphi_\epsilon|^2 + \frac{1}{\epsilon^2}\varphi_\epsilon^2 \right\} \leq C\epsilon \tag{1.4.21}$$

and check it by a straightforward computation. Indeed,

$$\begin{aligned} \int_B \left\{ |\nabla\varphi_\epsilon|^2 + \frac{1}{\epsilon^2}\varphi_\epsilon^2 \right\} &\leq \int_0^{2\pi} \mathrm{d}\theta \int_{1-\epsilon}^1 \mathrm{d}\rho \left\{ \frac{1}{\epsilon^2}\rho\,|\sigma_\epsilon(\theta)|^2 + \frac{1}{\rho}\,|\sigma_\epsilon'(\theta)|^2 + \rho\,|\sigma_\epsilon(\theta)|^2 \right\} \\ &\leq \frac{1}{\epsilon^2}\left(\epsilon - \frac{\epsilon^2}{2}\right) \|\sigma_\epsilon\|^2_{L^2(\mathbb{S}^1)} - \log(1-\epsilon)\,\|\sigma_\epsilon'\|^2_{L^2(\mathbb{S}^1)} + \left(\epsilon - \frac{\epsilon^2}{2}\right)\|\sigma_\epsilon\|^2_{L^2(\mathbb{S}^1)} \end{aligned}$$

and (1.4.21) follows from (1.4.19), since $|\sigma_\epsilon'| \leq |\nabla(v_\epsilon - \pi(v_\epsilon))|$ and $\sigma_\epsilon^2 \leq Cf(v_\epsilon)$.

Step 3 (Construction of a normal field on $\mathscr{N}$). By construction, $(v_\epsilon - \omega_\epsilon)_{|\partial B}$ is a normal field on $\mathscr{N}$, whose modulus is given by σ_ϵ. We want to extend it to a map $\nu_\epsilon \colon B \to \mathbb{R}^d$, so that $\nu_\epsilon(x)$ is orthogonal to $\mathscr{N}$ at the point $\omega_\epsilon(x)$ and $|\nu_\epsilon(x)| = \varphi_\epsilon(x)$, for all $x \in D$. At first, one may work locally, near a point $x_0 \in \partial\Omega$, and exploit the existence of an orthonormal frame of normal vectors, defined on some neighborhood of $\omega_\epsilon(x_0)$. Then, the construction of ν_ϵ is completed by a partition of the unity argument.

Step 4 (Construction of a comparison map). Set $\tilde\omega_\epsilon := \omega_\epsilon + \nu_\epsilon$. It follows from the previous steps that $\tilde\omega_\epsilon$ enjoys these properties:

$$\tilde\omega_{\epsilon|\partial B} = v_{\epsilon|\partial B},$$
$$\pi(\tilde\omega_\epsilon(x)) = v_\epsilon(x) \quad \text{and} \quad \mathrm{dist}(\tilde\omega_\epsilon(x),\,\mathscr{N}) = \varphi_\epsilon(x) \quad \text{for all } x \in B.$$

In particular, $\tilde\omega_\epsilon$ is an admissible comparison map for v_ϵ. By this information and Lemma 1.2.3, we infer a bound for the gradient of $\tilde\omega_\epsilon$:

$$|\nabla\tilde\omega_\epsilon|^2 \leq (1 + C\varphi_\epsilon)\,|\nabla\omega_\epsilon|^2 + C\left(|\nabla\varphi_\epsilon|^2 + \varphi_\epsilon^2\right)$$

Since $|\varphi_\epsilon| \leq \delta$ by construction, integrating this inequality over D and exploiting (1.4.19) we obtain

$$\|\nabla\tilde\omega_\epsilon\|^2_{L^2(D)} \leq (1+\delta)\,\|\nabla\omega_\epsilon\|^2_{L^2(D)} + C\epsilon. \tag{1.4.22}$$

The potential energy of $\tilde\omega_\epsilon$ is estimated by means of Remark 1.2.4:

$$\frac{1}{\epsilon^2}\int_B f(\tilde\omega_\epsilon) \leq \frac{M_0}{2\epsilon^2}\int_B \varphi_\epsilon^2.$$

Combining this inequality with (1.4.21) and (1.4.22), we deduce

$$\int_B e_\epsilon(v_\epsilon) \leq \int_B e(\tilde\omega_\epsilon) \leq (1+\delta)\,\|\nabla\omega_\epsilon\|^2_{L^2(D)} + C\epsilon. \tag{1.4.23}$$

With this estimate and (1.4.20), we complete the proof. □

Having established all these preliminary results, Proposition 1.4.4 follows easily from a covering argument as, for instance, the one in [12] (see also [14, Chapter IV]).

Proof of Proposition 1.4.4. By Vitali covering lemma, we can find a finite family of points $\{y_i\}_{i\in I}$ such that

$$\Omega \subseteq \bigcup_{i\in I} B(y_i,\, 3\varepsilon^{\alpha/2})$$

and

$$B(y_i,\, \varepsilon^{\alpha}) \cap B(y_j,\, \varepsilon^{\alpha}) = \emptyset \qquad \text{if } i \neq j.$$

Let $\eta_\alpha = \eta_\alpha(\alpha,\, \delta)$ be given by Proposition 1.4.10. Define J_ε as the subset of indexes $i \in I$ for which the inequality

$$\int_{B(y_i,\, 3\varepsilon^{\alpha/2})} |\nabla u_\varepsilon|^2 \geq \eta_\alpha \left(|\log \varepsilon| + 1\right)$$

holds. Then, by Lemma 1.4.3, we have

$$\eta_\alpha \left(|\log \varepsilon| + 1\right) \mathrm{card}(J_\varepsilon) \leq \sum_{j\in J_\varepsilon} \int_{B(y_i,\, 3\varepsilon^{\alpha/2})} |\nabla u_\varepsilon|^2 \leq C \left(|\log \varepsilon| + 1\right) \tag{1.4.24}$$

(to prove the last inequality, recall that there is a universal constant C such that each point of Ω is covered by at most C balls of radius $3\varepsilon^{\alpha/2}$). It follows that $\mathrm{card}(J_\varepsilon)$ is bounded independently of ε. Moreover, Propositions 1.4.9 and 1.4.10 imply that

$$\begin{aligned} \mathrm{dist}(u_\varepsilon(x),\, \mathscr{N}) \leq \delta \qquad & \text{if } x \in B(y_i,\, 3\varepsilon^{\alpha/2})\text{and } i \in I \setminus J_\varepsilon \\ \varepsilon^{4\alpha} e_\varepsilon(u_\varepsilon)(x) \leq C_\alpha \qquad & \text{if } x \in B(y_i,\, \varepsilon^{\alpha})\text{and } i \in I \setminus J_\varepsilon. \end{aligned}$$

Now, let us fix an index $i \in J_\varepsilon$, and let us focus on $B(y_i,\, 3\varepsilon^{\alpha/2})$. Being $\lambda_0 = \lambda_0(\delta)$ and $\mu_0 = \mu_0(\delta)$ given by Proposition 1.4.6, we consider a finite covering $\{B(x^i_m,\, 3\lambda_0\varepsilon)\colon m \in \Lambda_{\varepsilon,\, i}\}$ of $B(y_i,\, 3\varepsilon^{\alpha/2})$, such that

$$B(x^i_m,\, \lambda_0\varepsilon) \cap B(x^i_n,\, \lambda_0\varepsilon) = \emptyset \qquad \text{if } m \neq n,$$

and we define the set $L_{\varepsilon,\, i}$ of indexes $m \in \Lambda_{\varepsilon,\, i}$ such that

$$\frac{1}{\varepsilon^2} \int_{B(x^i_m,\, 3\lambda_0\varepsilon)} f(u_\varepsilon) > \mu_0.$$

Since $\varepsilon^{-2} \int_{B(x_i,\, 3\varepsilon^{\alpha/2})} f(u_\varepsilon)$ is controlled by Lemma 1.4.8, we can bound the cardinality of $L_{\varepsilon,\, i}$, independently of ε, exactly as in (1.4.24). By Proposition 1.4.6, we have that $\mathrm{dist}(u_\varepsilon(x),\, \mathscr{N}) \leq \delta$ if $x \in B(x^i_m,\, 3\lambda_0\varepsilon)$ and $m \notin L_{\varepsilon,\, i}$ Combining all these facts, we conclude easily. $\square$

Denote by $x^\varepsilon_1,\, x^\varepsilon_2, \ldots,\, x^\varepsilon_{k_\varepsilon}$ the elements of X_ε. For any given sequence $\varepsilon_n \searrow 0$ we can extract a renamed subsequence, such that k_{ε_n} is independent of n (say, $k_{\varepsilon_n} = N'$) and

$$x^{\varepsilon_n}_i \to L_i \qquad \text{for } \ i \in \{1,\, 2,\, \ldots,\, N'\},$$

for some point $L_i \in \overline{\Omega}$ Some of the points L_i might coincide. Therefore, we relabel them as $a_1,\, a_2,\, \ldots,\, a_N$, with $N \leq N'$, in such a way that $a_i \neq a_j$ if $i \neq j$.

For the time being, we cannot exclude the possibility that $a_i \in \partial\Omega$, for some index i. To deal with this difficulty, we enlarge a little the domain Ω and consider a smooth, bounded domain $\Omega' \supseteq \Omega$, with the same homotopy type as Ω — for instance, we can define Ω' as a r-neighborhood of Ω, for r small enough. Also, we fix a smooth function $\bar{g}\colon \Omega' \setminus \Omega \to \mathscr{N}$, such that $\bar{g} = g$ on $\partial\Omega$ and $\|\nabla \bar{g}\|_{L^2(\Omega'\setminus\Omega)} \leq C\, \|g\|_{H^1(\partial\Omega)}$. From now on, we extend systematically any function $v\colon \Omega \to \mathscr{N}$ with $v = g$ on $\partial\Omega$ to a map $\bar{v}\colon \Omega' \to \mathscr{N}$, by setting $\bar{v} = \bar{g}$ on $\Omega' \setminus \Omega$.

1.4.2 An upper estimate away from singularities

Fix a number $\rho > 0$ small enough, say,

$$\rho < \operatorname{dist}(\Omega, \Omega'), \qquad \rho < \frac{1}{2}\min_{i\neq j}|a_i - a_j|,$$

so that the disks $B(a_i, \rho)$ are mutually disjoint and contained in Ω'. The aim of the following subsection is to prove the following upper bound for energy of the minimizers, away from the singularities.

Proposition 1.4.12. *There exists a constant C, independent of n and ρ, and a number N_ρ such that for every $n \geq N_\rho$ we have*

$$\frac{1}{2}\int_{\Omega'\setminus\bigcup_i B(a_i,\rho)} |\nabla u_{\varepsilon_n}|^2 \leq \kappa_* |\log\rho| + C.$$

Before facing the proof, we fix some notations. For a fixed i, define Λ_i as the set of indexes $j \in \{1, 2, \ldots, N_1\}$ such that $x_j^{\varepsilon_n} \to a_i$. For n sufficiently large, we have $B(a_i, \rho) \supseteq B(x_j^{\varepsilon_n}, \lambda_0\varepsilon_n)$ if and only if $j \in \Lambda_i$. We introduce the sets

$$\Omega_{i,n} := B(a_i, \rho) \setminus \bigcup_{j\in\Lambda_i} B(x_j^{\varepsilon_n}, \lambda_0\varepsilon_n).$$

Recall that, by Proposition 1.4.4, we have $\operatorname{dist}(u_{\varepsilon_n}(x), \mathscr{N}) \leq \delta$ for all $x \in \Omega_{i,n}$. Thus, we can define v_{ε_n}, σ_{ε_n} by

$$v_{\varepsilon_n} := \pi(u_{\varepsilon_n|\Omega_{i,n}}), \qquad \sigma_{\varepsilon_n} := \operatorname{dist}(u_{\varepsilon_n|\Omega_{i,n}}, \mathscr{N}).$$

and notice that $v_{\varepsilon_n}, \sigma_{\varepsilon_n} \in H^1(\Omega_{i,n}, \mathscr{N})$. Denote by $\eta_{j,n}$ the free homotopy class of v_{ε_n}, restricted to $\partial B(x_j^{\varepsilon_n}, \lambda_0\varepsilon_n)$, and set

$$\kappa_{i,n} := \inf\Big\{\lambda_*(\gamma)\colon \gamma \in \prod_{j\in\Lambda_i}\eta_{j,n}\Big\},$$

The continuity of v_{ε_n} and Lemma 1.2.1 imply

$$\prod_{j=1}^{N_1}\eta_{j,n} \cap \prod_{i=1}^{k}\gamma_i \neq \emptyset.$$

By the definition (1.2.9) of κ_* we infer

$$\kappa_* \leq \sum_{i=1}^{N}\kappa_{i,n}, \qquad \text{for all } n \in \mathbb{N}. \tag{1.4.25}$$

We can assume without loss of generality that $\kappa_{i,n} > 0$ for all i, n. Indeed, if $\kappa_{i,n} = 0$ then there is no topological obstruction to the construction of Lemma 1.4.11. Arguing in a similar way, we can exhibit a comparison map $\tilde{u}_{\varepsilon_n}$, with $\tilde{u}_{\varepsilon_n|\partial B(a_i,\rho)} = u_{\varepsilon_n|\partial B(a_i,\rho)}$, such that

$$E_\varepsilon(u_{\varepsilon_n}, B(a_i, \rho)) \leq E_\varepsilon(\tilde{u}_{\varepsilon_n}, B(a_i, \rho)) \leq C.$$

Applying the Chen and Struwe's result on some small ball contained in $B(a_i, \rho)$, we obtain $e_\varepsilon(u_\varepsilon) \leq C$ on $B(a_i, \rho)$. In turns, this forces

$$\operatorname{dist}^2(u_{\varepsilon_n}(x), \mathscr{N}) \leq Cf(u_{\varepsilon_n}(x)) \leq C\varepsilon_n^2 \leq \delta,$$

for all $x \in B(a_i, \rho)$ and n large enough. Therefore, no singularity is contained in $B(a_i, \rho)$ if $\kappa_{i,n} = 0$, and the point a_i can be dropped out.

After this preliminaries, we are ready to face the proof of Proposition 1.4.12. In fact, we will give an indirect proof, based on a lower estimate for the energy near the singularities.

Lemma 1.4.13. *There exists a constant C, independent of n and ρ, such that for all function $v \in H^1(\Omega_{i,n}, \mathscr{N})$ the estimate*

$$\frac{1}{2}\int_{\Omega_{i,n}} |\nabla v|^2 \geq \kappa_{i,n}\left(\log\frac{\rho}{\varepsilon_n} - C\right)$$

holds.

Sketch of the proof. The lemma can be established arguing exactly as in [123, Theorem 1] (the reader is also referred to [33]). At first, one has to consider the case $\Omega_{i,n}$ is an annulus $B_\rho \setminus B_\varepsilon$, with $0 < \varepsilon < \rho$: then, $\kappa_{i,n}$ reduces to $\lambda_*(\eta)$, where η is the homotopy class of $v_{|\partial B_\rho}$. Assuming that v is smooth, a computation in polar coordinates gives

$$\frac{1}{2}\int_{B_\rho\setminus B_\varepsilon} |\nabla v|^2 = \frac{1}{2}\int_\varepsilon^\rho \mathrm{d}r \int_0^{2\pi} \mathrm{d}\theta \left\{ r\left|\frac{\partial v}{\partial r}\right|^2 + \frac{1}{r}\left|\frac{\partial v}{\partial \theta}\right|^2 \right\} \geq \frac{1}{2}\int_\varepsilon^\rho \frac{\mathrm{d}r}{r}\int_0^{2\pi}\mathrm{d}\theta\left|\frac{\partial v}{\partial\theta}\right|^2$$

and, since the definition (1.2.6) of λ implies

$$2\pi\int_0^{2\pi}\left|\frac{\partial v}{\partial\theta}\right|^2 \mathrm{d}\theta \geq \lambda^2(\eta),$$

we deduce

$$\frac{1}{2}\int_{B_\rho\setminus B_\varepsilon} |\nabla v|^2 \geq \frac{\lambda^2(\eta)}{4\pi}\log\frac{\rho}{\varepsilon} \geq \lambda_*(\eta)\log\frac{\rho}{\varepsilon}. \tag{1.4.26}$$

Having proved the lemma in this simple case, we can repeat the same argument as [123], the only difference being $\kappa_{i,n}$ in place of the degree. We exploit the property (1.2.8) instead of the triangle inequality for the degrees. Finally, since we may assume

$$\mathrm{dist}(B(x_j^{\varepsilon_n}, \lambda_0\varepsilon_n), \partial B(a_i, \rho)) > \rho/2$$

for $j \in \Lambda_i$ and n large enough, we can prove the analogous of [123, Proposition], which reads

$$\frac{1}{2}\int_{\Omega_{i,n}} |\nabla v|^2 \geq \kappa_{i,n}\log\left(\frac{\rho/4}{\lambda_0\varepsilon_n}\right).$$

This concludes the proof. □

Lemma 1.4.14. *There exists a constant C, independent of n and ρ, and a number N_ρ such that for every $n \geq N_\rho$ and every i we have*

$$\frac{1}{2}\int_{\Omega_{i,n}} |\nabla u_{\varepsilon_n}|^2 \geq \kappa_{i,n}\left(\log\frac{\rho}{\varepsilon_n} - C\right) - C.$$

Proof. The energy of v_{ε_n} on $\Omega_{i,n}$ is bounded by below by Lemma 1.4.13. Moreover, the lower bound provided by (1.2.11) entails

$$|\nabla u_{\varepsilon_n}|^2 \geq (1 - C\sigma_{\varepsilon_n})\,|\nabla v_{\varepsilon_n}|^2.$$

If we knew

$$\int_{\Omega_{i,n}} \sigma_{\varepsilon_n}\,|\nabla v_{\varepsilon_n}|^2 \leq C, \tag{1.4.27}$$

then the lemma would follow. Therefore, let us introduce the set

$$Y_n := \{x \in \Omega\colon\ \mathrm{dist}(x, X_{\varepsilon_n}) \leq \varepsilon_n^\alpha\}$$

and split the proof of (1.4.27) in two cases.

Case 1 (Estimate out of Y_n). Let $x \in \Omega_{i,n} \setminus Y_n$. Then, by Propositions 1.4.4 and 1.4.10 we have

$$e_{\varepsilon_n}(u_{\varepsilon_n})(x) \leq C_\alpha \varepsilon_n^{4\alpha}.$$

Since $|\nabla v_{\varepsilon_n}| \leq C\,|\nabla u_{\varepsilon_n}|$, this entails

$$\int_{\Omega_{i,n}} \sigma_{\varepsilon_n} |\nabla v_{\varepsilon_n}|^2 \leq C \int_{\Omega_{i,n}} \sigma_{\varepsilon_n} |\nabla u_{\varepsilon_n}|^2 \leq C\varepsilon_n^{1-6\alpha}$$

which implies (1.4.27) if we choose $\alpha < 1/6$.
Case 2 (Estimate on Y_n). We apply the Hölder inequality:

$$\int_{Y_n} \sigma_{\varepsilon_n} |\nabla v_{\varepsilon_n}|^2 \leq C \int_{Y_n} \sigma_{\varepsilon_n} |\nabla u_{\varepsilon_n}|^2 \leq C \, \|\sigma_{\varepsilon_n}\|_{L^2(Y_n)} \|\nabla u_{\varepsilon_n}\|^2_{L^4(Y_n)} \,. \tag{1.4.28}$$

The norm of the gradient is estimated by the Gagliardo-Niremberg interpolation inequality and standard elliptic regularity results. We obtain

$$\|\nabla u_{\varepsilon_n}\|_{L^4(Y_n)} \leq C \, \|\Delta u_{\varepsilon_n}\|^{1/2}_{L^2(Y_n)} \|u_{\varepsilon_n}\|^{1/2}_{L^\infty(Y_n)} \,,$$

which reduces to

$$\|\nabla u_{\varepsilon_n}\|_{L^4(Y_n)} \leq C\varepsilon_n^{-1} \, \|\nabla_u f(u_{\varepsilon_n})\|^{1/2}_{L^2(Y_n)} \tag{1.4.29}$$

since u_{ε_n} verifies the Equation (1.2.1) and its L^∞ norm is bounded by Lemma 1.4.1. For a fixed $v \in \mathscr{N}$, a Taylor expansion of f around the point $\pi(v)$ (see Remark 1.2.4) yields

$$|\mathrm{D}f(v)| \leq M_0 \,\mathrm{dist}(v, \, \mathscr{N}). \tag{1.4.30}$$

Thus, combining the Equations (1.4.28), (1.4.29) and (1.4.30) with (H_2), we infer

$$\int_{Y_n} \sigma_{\varepsilon_n} |\nabla v_{\varepsilon_n}|^2 \leq C\varepsilon_n^{-2} \, \|\sigma_{\varepsilon_n}\|^2_{L^2(Y_n)} \leq M_0 \varepsilon_n^{-2} \int_{Y_n} f(u_{\varepsilon_n}).$$

Finally, since Y_n is a finite union of balls of radius ε^α, Lemma 1.4.8 implies the desired estimate (1.4.27), for a constant depending on α. $\square$

Proposition 1.4.12 follows now easily from Lemmas 1.4.3 and 1.4.14, with the help of (1.4.25). Let us point out some consequences of the previous results. For a fixed a compact set $K \subseteq \Omega' \setminus \{a_i\}_{1 \leq i \leq N}$, we know by Proposition 1.4.12 that

$$\frac{1}{2} \int_K |\nabla u_{\varepsilon_n}|^2 \leq C_K, \qquad \int_K \mathrm{dist}^2(u_{\varepsilon_n}, \, \mathscr{N}) \leq C\varepsilon_n^2 \tag{1.4.31}$$

at least for $n \geq N_K$. Hence, up to a renamed subsequence, by a diagonal procedure we can assume

$$u_{\varepsilon_n} \to u_0 \qquad \text{a.e. and weakly in } H^1_{\mathrm{loc}}(\Omega' \setminus \{a_1, \, \ldots, \, a_N\}).$$

Passing to the limit in the second condition of (1.4.31), by Fatou lemma we deduce that

$$u_0(x) \in \mathscr{N} \qquad \text{for a.e. } x \in \Omega' \setminus \{a_1, \, \ldots, \, a_N\}.$$

We are now in position to prove that the points a_i, for $i \in \{1, \, \ldots, \, N\}$, do not belong to the boundary of Ω. As a byproduct of the proof, we obtain a condition for the quantities $\kappa_{i,n}$.

Proposition 1.4.15. *For all $i \in \{1, \, \ldots, \, N\}$, the point a_i is in the interior of Ω. In addition, it holds that*

$$\sum_{i=1}^N \kappa_{i,n} = \kappa_*. \tag{1.4.32}$$

Proof. We adapt the proof of [14, Lemma 3] (the reader may see also [33]). Assume, by contradiction, that $a_i = 0 \in \partial\Omega$ for some $i \in \{1, \ldots, N\}$. Then, computing in polar coordinates as we did in Lemma 1.4.13, we obtain the inequality

$$\frac{1}{2}\int_{\Omega\cap(B_\rho\setminus B_\varepsilon)} |\nabla u_0|^2 \geq \frac{\lambda^2(\eta)}{2\pi}(1+\mathrm{o}_{\rho\to 0}(1))\log\frac{\rho}{\varepsilon}$$

in place of (1.4.26). The factor approximately equal to $(2\pi)^{-1}$, instead of $(4\pi)^{-1}$, is due to the angular variable, which spans an interval of length $\pi + o_{\rho\to 0}(1)$. Arguing as in [123, Theorem], we can conclude

$$\frac{1}{2}\int_{\Omega\setminus\cup_i B(a_i,\,\rho)} |\nabla u_0|^2 \geq \left(\sum_{i=1}^N \alpha_i\kappa_{i,n}\right)(1+o_{\rho\to 0}(1))\,|\log\rho| - C \tag{1.4.33}$$

for a radius $\rho > 0$ small enough, so that the balls $B(a_i,\,\rho)$ are mutually disjoint, and the coefficients α_i are given by

$$\alpha_i := \begin{cases} 1 & \text{if } a_i \notin \partial\Omega \\ 2 & \text{if } a_i \in \partial\Omega. \end{cases}$$

On the other hand, the weak H^1_{loc} convergence of u_{ε_n} and Proposition 1.4.12 imply

$$\frac{1}{2}\int_{\Omega\setminus\cup_i B(a_i,\,\rho)} |\nabla u_0|^2 \leq \liminf_{n\to+\infty} E_{\varepsilon_n}(u_{\varepsilon_n},\,\Omega\setminus\cup_i B(a_i,\,\rho)) \leq \kappa_*\,|\log\rho| + C. \tag{1.4.34}$$

Combining (1.4.33) and (1.4.34), dividing by $|\log\rho|$ then passing to the limit as $\rho\to 0$, we deduce

$$\sum_{i=1}^N \alpha_i\kappa_{i,n} \leq \kappa_*.$$

In view of the inequality (1.4.25), we have

$$\sum_{i=1}^N \alpha_i\kappa_{i,n} = \kappa_*$$

and, since $\kappa_{i,n} > 0$ for all i and n, it must be $\alpha_i = 1$ for all i, that is, the points a_i do not belong to the boundary. The equality (1.4.32) also follows. ☐

1.4.3 Proof of Theorem 1.1.3

The proof is, essentially, a refined version of the argument we used for Proposition 1.4.10. Since the result we want to prove is local, we fix a closed disk $D \subseteq \Omega' \setminus \{a_1, \ldots, a_N\}$ and restrict our attention to D. In what follows, we assume that $D \subseteq \Omega$, for ease of notation. In case D intersect the boundary of Ω, the following argument can be modified in a straightforward way.

By Proposition 1.4.12, and changing the radius of the disk if necessary, we can assume that

$$\int_{\partial D}\left\{\frac{1}{2}|\nabla u_{\varepsilon_n}|^2 + \frac{1}{\varepsilon_n^2}f(u_{\varepsilon_n})\right\}\mathrm{d}\mathscr{H}^1 \leq C. \tag{1.4.35}$$

This is always possible, up to a subsequence. Indeed, denoting by a, R the center and the radius of D, by Fatou lemma we have

$$\int_0^R \mathrm{d}\rho \liminf_{n\to+\infty}\int_{\partial B(a,\,\rho)} \mathrm{d}\mathscr{H}^1\left\{\frac{1}{2}|\nabla u_{\varepsilon_n}|^2 + \frac{1}{\varepsilon_n^2}f(u_{\varepsilon_n})\right\} \leq \liminf_{n\to+\infty} E_{\varepsilon_n}(u_{\varepsilon_n},\,D) \leq C.$$

Hence, clearly it exists $\bar{\rho} \in (0, R)$ such that

$$\liminf_{n \to +\infty} \int_{\partial B(a, \bar{\rho})} \left\{ \frac{1}{2} |\nabla u_{\varepsilon_n}|^2 + \frac{1}{\varepsilon_n^2} f(u_{\varepsilon_n}) \right\} \mathrm{d}\mathscr{H}^1 \leq C.$$

Due to the compact inclusion $H^1(\partial D) \hookrightarrow C^0(\partial D)$, we have the uniform convergence $u_{\varepsilon_n} \to u_0$ on ∂D. We perform the same construction of Lemma 1.4.11, and we obtain a sequence $\omega_{\varepsilon_n} : D \to \mathscr{N}$ of minimizing harmonic maps, and another sequence $\tilde{\omega}_{\varepsilon_n} : D \to \mathbb{R}^d$ such that

$$\omega_{\varepsilon_n | \partial D} = \pi(u_{\varepsilon_n})_{|\partial D}, \qquad \tilde{\omega}_{\varepsilon_n | \partial D} = u_{\varepsilon_n | \partial D}$$

and

$$E_{\varepsilon_n}(\tilde{\omega}_{\varepsilon_n}, D) \leq \frac{1}{2} (1 + o_{n \to +\infty}(1)) \|\nabla \omega_{\varepsilon_n}\|^2_{L^2(D)} + C\varepsilon_n \tag{1.4.36}$$

(compare with (1.4.22), (1.4.23)). The functions ω_{ε_n} are bounded in $H^1(D)$ since u_{ε_n} are (by (1.4.35)), hence we can apply the strong compactness result [61, Theorem 5.3] and deduce, up to subsequences,

$$\omega_{\varepsilon_n} \to \omega_0 \qquad \text{strongly in } H^1(D), \tag{1.4.37}$$

where ω_0 is a minimizing harmonic map. Passing to the limit in the boundary condition for ω_{ε_n}, we see that $\omega_{0|\partial D} = u_{0|\partial D}$. As $\{u_{\varepsilon_n}\}_{n \in \mathbb{N}}$ converges weakly in $H^1(D)$, we deduce

$$\frac{1}{2} \|\nabla u_0\|^2_{L^2(D)} \leq \frac{1}{2} \liminf_{n \to +\infty} \|\nabla u_{\varepsilon_n}\|^2_{L^2(D)}$$

but, on the other hand, (1.4.36) and (1.4.37) give

$$\frac{1}{2} \limsup_{n \to +\infty} \|\nabla u_{\varepsilon_n}\|^2_{L^2(D)} \leq \limsup_{n \to +\infty} E_{\varepsilon_n}(u_{\varepsilon_n}, D) \leq \frac{1}{2} \|\nabla \omega_0\|^2_{L^2(D)} \leq \frac{1}{2} \|\nabla u_0\|^2_{L^2(D)}.$$

These inequalities, combined, yield

$$\lim_{n \to +\infty} \|\nabla u_{\varepsilon_n}\|_{L^2(D)} = \frac{1}{2} \|\nabla u_0\|^2_{L^2(D)} = \frac{1}{2} \|\nabla \omega_0\|^2_{L^2(D)}.$$

As a consequence, the convergence $u_{\varepsilon_n} \to u_0$ holds in $H^1(D)$ and the limit map u_0 is minimizing harmonic. In particular, u_0 solves the harmonic map equation in D, and the regularity theory of Morrey (see [105]) applies, entailing $u_0 \in C^\infty(D)$. Also, as a byproduct of this argument, we obtain

$$\frac{1}{\varepsilon_n^2} \int_D f(u_{\varepsilon_n}) \to 0 \qquad \text{as } n \to +\infty. \tag{1.4.38}$$

Finally, we check the locally uniform convergence. Owning to the strong convergence in $H^1(D)$ and (1.4.38), for all $\eta > 0$ we can find a radius $r > 0$, such that the inequality

$$\int_{B(x_0, r)} e_{\varepsilon_n}(u_{\varepsilon_n}) \leq \eta$$

holds for all $x_0 \in \frac{1}{2}D$ and all $n \in \mathbb{N}$. Then, choosing η small enough, we apply the Chen and Struwe's result, to infer

$$e_{\varepsilon_n}(u_{\varepsilon_n})(x_0) \leq E_{\varepsilon_n}(u_{\varepsilon_n}, D) \leq C \qquad \text{for all } x \in \frac{1}{2}D.$$

This provides a bound for u_{ε_n} in $W^{1,\infty}(D)$, which allows us to conclude the proof, by means of the Ascoli-Arzelà theorem.

1.5 The behaviour of u_0 near the singularities

In this section, we analyze the behaviour of u_0 near the singularities: our aim is to prove Proposition 1.1.4. We consider here just the case $\mathscr{N} = \mathbb{RP}^2$. This provide a remarkable simplification in the arguments, due to the simple homotopic structure of the real projective plane, whose fundamental group consists of two elements only. Hence, there is a unique class of homotopically non-trivial loops. This property reflects on the structure of the limit map. Remind that, for all i and n, we have set

$$\kappa_{i,n} = \lambda_* \left(\prod_{j \in \Lambda_i} \eta_{j,n} \right),$$

where $\eta_{j,n}$ is the free homotopy class of $\pi(u_{\varepsilon_n})$, restricted to $\partial B(x_j^{\varepsilon_n},\, \lambda_0 \varepsilon_n)$. It follows from Lemma 1.2.1 that $\prod_{j \in \Lambda_i} \eta_{j,n}$ is the homotopy class of $\pi(u_{\varepsilon_n})$ restricted to $\partial B(a_i,\, \rho)$, for a small radius $\rho > 0$. Since the homotopy class is stable by uniform convergence, from Theorem 1.1.3 we deduce

$$\kappa_{i,n} = \lambda_* \left(\text{homotopy class of } u_{0|\partial B(a_i,\, \rho)}\right),$$

that is, $\kappa_{i,n}$ is independent of n. On the other hand, there is a unique non zero value that $\kappa_{i,n}$ and κ_* can assume, corresponding to the unique class of non-trivial loops. As a consequence, from (1.4.32) we infer that that there is at most one index i such that $\kappa_{i,n} \neq 0$, and we prove the following

Lemma 1.5.1. *In case $\mathscr{N} \simeq \mathbb{RP}^2$, there exists a point $a \in \Omega$ such that $u_0 \in C^\infty(\Omega \setminus \{a\})$.*

Assume now that the boundary datum is homotopically non-trivial. Up to a translation, we can suppose that the unique singular point of u_0 is the origin, and we fix a radius $r > 0$ such that $B(0,\, r) \subseteq \Omega$. We also introduce the functions $R, S \in C^\infty(0,\, r)$ by

$$R(\rho) := \frac{1}{2} \int_{\partial B_\rho} \left| \frac{\partial u_0}{\partial \nu} \right|^2 \, \mathrm{d}\mathscr{H}^1$$

and

$$S(\rho) := \frac{1}{2\rho} \int_{\partial B_\rho} \left| \nabla_\top u_0 \right|^2 \, \mathrm{d}\mathscr{H}^1$$

where $\nabla_\top$ denotes the tangential derivation. These functions are obviously non negative; in fact, S is bounded by below by κ_*. Indeed, by definition of λ we have for all $\rho \in (0,\, r)$

$$4\pi S(\rho) = 2\pi \int_0^{2\pi} \left| c'_\rho(\theta) \right|^2 \, \mathrm{d}\theta \geq \lambda^2(\gamma),$$

where c_ρ is the function considered in Proposition 1.1.3, and

$$S(\rho) \geq \frac{\lambda^2(\gamma)}{4\pi} = \kappa_*.$$

Lemma 1.5.2. *The function $\rho \mapsto \rho^{-1}(S(\rho) - \kappa_*)$ is summable over $(0,\, r)$. In particular,*

$$\liminf_{\rho \to 0} S(\rho) = \kappa_*.$$

Proof. Let $0 < \rho_0 < \min\{r,\, 1\}$. With the help of Theorem 1.1.3, we can pass to the limit as $n \to +\infty$ in Proposition 1.4.12, to obtain

$$\frac{1}{2} \int_{B_r(0) \setminus B_{\rho_0}(0)} \left| \nabla u_0 \right|^2 \leq \kappa_* \left| \log \rho_0 \right| + C$$

and, expressing the left-hand side in polar coordinates,

$$\int_{\rho_0}^{r} \left\{ R(\rho) + \frac{1}{\rho} S(\rho) \right\} \mathrm{d}\rho \leq \kappa_* \left|\log \rho_0\right| + C. \tag{1.5.1}$$

Taking advantage of this bound, we compute

$$\int_{\rho_0}^{r} \frac{1}{\rho} \left(S(\rho) - \kappa_*\right) \mathrm{d}\rho = \int_{\rho_0}^{r} \frac{S(\rho)}{\rho} \mathrm{d}\rho - \kappa_* \left|\log \rho_0\right| - \kappa_* \log r \leq C.$$

Letting $\rho_0 \searrow 0$, we deduce the summability of $\rho \mapsto \rho^{-1}(S(\rho) - \kappa_*)$ which, in turns, forces the inferior limit of $S - \kappa_*$ to vanish. ☐

Proposition 1.1.4 follows easily from this lemma. Indeed, we can pick a sequence $\rho_n \searrow 0$ such that $S(\rho_n) \to \kappa_*$: this is a minimizing sequence for the length-squared functional

$$c \in H^1(\mathbb{S}^1, \mathscr{N}) \mapsto \frac{1}{2} \int_0^{2\pi} \left|c'(\theta)\right|^2 \mathrm{d}\theta$$

under the constraint that c is homotopically non-trivial, and hence, by compact inclusion $H^1(\mathbb{S}^1, \mathscr{N}) \hookrightarrow C^0(\mathbb{S}^1, \mathscr{N})$, it admits a subsequence uniformly converging to a minimizer, which is a geodesic. The continuous inclusion $H^1(\mathbb{S}^1, \mathscr{N}) \hookrightarrow C^{1/2}(\mathbb{S}^1, \mathscr{N})$ and interpolation in Hölder spaces provide also the convergence in C^α, for $\alpha \in (0, 1/2)$.

We are not able to say whether the convergence holds for the whole family $\{c_\rho\}_{\rho > 0}$, because we are not able to identify the limit geodesic c_ρ. However, we state here some additional properties we have been able to prove about the functions S and R, in the hope that they might be of interest for future work.

Lemma 1.5.3. *It holds that*

$$R(\rho) = \frac{1}{\rho} \left(S(\rho) - \kappa_*\right).$$

Proof. We claim that

$$\frac{\mathrm{d}}{\mathrm{d}\rho} \left(\rho R(\rho) - S(\rho)\right) = 0. \tag{1.5.2}$$

This equality is essentially a consequence of the Pohozaev identity for the harmonic maps, but here we will present its proof in a slightly different form. Since u_0 is harmonic away from 0, the Laplace operator Δu_0 is, at every point, a normal vector to $\mathscr{N}$. Thus, for each point $x \in \Omega \setminus \{0\}$ we have

$$\left(\Delta u_0 \cdot \frac{\partial u_0}{\partial \nu}\right)(x) = 0,$$

where $\nu = x / |x|$. We multiply the previous identity by $|x|^2$, pass to polar coordinates, and integrate with respect to $\theta \in [0, 2\pi]$, for a fixed $\rho \in [0, r]$. This yields

$$\rho^2 \int_0^{2\pi} \frac{\partial^2 u_0}{\partial \rho^2} \cdot \frac{\partial u_0}{\partial \rho} \mathrm{d}\theta + \rho \int_0^{2\pi} \left|\frac{\partial u_0}{\partial \rho}\right|^2 \mathrm{d}\theta + \int_0^{2\pi} \frac{\partial^2 u_0}{\partial \theta^2} \cdot \frac{\partial u_0}{\partial \rho} \mathrm{d}\theta = 0$$

and, after an integration by parts in the third term,

$$\frac{\rho^2}{2} \frac{\mathrm{d}}{\mathrm{d}\rho} \int_0^{2\pi} \left|\frac{\partial u_0}{\partial \rho}\right|^2 \mathrm{d}\theta + \rho \int_0^{2\pi} \left|\frac{\partial u_0}{\partial \rho}\right|^2 \mathrm{d}\theta - \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}\rho} \int_0^{2\pi} \left|\frac{\partial u_0}{\partial \theta}\right|^2 \mathrm{d}\theta = 0.$$

This equality can be rewritten as

$$\rho^2 \frac{\mathrm{d}}{\mathrm{d}\rho} \left(\frac{R(\rho)}{\rho}\right) + 2R(\rho) - \frac{\mathrm{d}}{\mathrm{d}\rho} S(\rho) = 0,$$

from which we deduce (1.5.2). Our claim is proved.

As a consequence of (1.5.2), there exists a constant k such that

$$R(\rho) = \frac{1}{\rho}\left(S(\rho) + k\right),$$

and the lemma will be proved once we have identified the value of k. To do so, fix $0 < \rho_0 < \min\{r, 1\}$ and notice that (1.5.1) implies

$$\kappa_* \left|\log \rho_0\right| + C \geq \int_{\rho_0}^{r} \frac{1}{\rho}\left(2S(\rho) + k\right) \,\mathrm{d}\rho = \int_{\rho_0}^{r} \frac{2}{\rho}\left(S(\rho) - \kappa_*\right) \,\mathrm{d}\rho + \int_{\rho_0}^{r} \frac{1}{\rho}(2\kappa_* + k) \,\mathrm{d}\rho$$

The first integral at the right-hand side is non negative, since $S \geq \kappa_*$. Therefore, for small values of ρ_0,

$$\kappa_* \left|\log \rho_0\right| + C \geq (2\kappa_* + k) \left|\log \rho_0\right| - C$$

and, comparing the coefficients of the leading terms, we have $\kappa_* \geq 2\kappa_* + k$, that is, $k \leq -\kappa_*$. On the other hand,

$$0 \leq \rho R(\rho) = S(\rho) + k$$

and, taking the inferior limit as $\rho \searrow 0$, by Lemma 1.5.2 we infer $0 \leq \kappa_* + k$, which provides the opposite inequality $k \geq -\kappa_*$. ☐

Lemmas 1.5.2 and 1.5.3 combined imply that $R \in L^1(0, r)$.

Remark 1.5.1. If we knew that R has better integrability properties, for instance $R \in L^p$ for some $p > 1$ (or even $R^{1/2} \in L^{(2,1)}$), then we could conclude the convergence of the whole family $\{c_\rho\}_{\rho>0}$, at least in $L^1(\mathbb{S}^1, \mathscr{N})$. Indeed, applying the fundamental theorem of calculus, the Fubini-Tonelli theorem, and the Hölder inequality, we would obtain

$$\left\|c_{\rho_1} - c_{\rho_2}\right\|_{L^1(\mathbb{S}^1)} \leq \int_0^{2\pi} \mathrm{d}\theta \int_{\rho_1}^{\rho_2} \mathrm{d}\rho \left|\frac{\partial u_0}{\partial \rho}\right| \leq \int_{\rho_1}^{\rho_2} \mathrm{d}\rho (2\pi\rho)^{1/2} \left\{\int_0^{2\pi} \mathrm{d}\theta \left|\frac{\partial u_0}{\partial \rho}\right|^2\right\}^{1/2}$$

and hence

$$\left\|c_{\rho_1} - c_{\rho_2}\right\|_{L^1(\mathbb{S}^1)} \leq \int_{\rho_1}^{\rho_2} \left(\frac{4\pi R(\rho)}{\rho}\right)^{1/2} \mathrm{d}\rho,$$

where the right-hand side converges to zero as $\rho_1, \rho_2 \to 0$, again by the Hölder inequality. Thus, $\{c_\rho\}_{\rho>0}$ would be a Cauchy sequence in $L^1(\mathbb{S}^1, \mathscr{N})$.

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Défauts de ligne dans modèle de Landau-de Gennes en dimension trois lorsque la constante élastique tend vers zéro

Le présent travail porte sur l'étude du modèle variationnel de Landau-de Gennes dans des domaines bornés en dimension trois. En particulier, nous sommes intéressés au comportement asymptotique des minimiseurs, lorsque la constante élastique tend vers zéro. En supposant que l'énergie des minimiseurs diverge de façon au plus logarithmique, nous montrons qu'il existe un ensemble fermé et 1-rectifiable $\mathscr{S}_{\mathrm{line}}$ (le défaut de ligne), de longueur finie, tels que les minimiseurs convergent à une application localement harmonique, loin de $\mathscr{S}_{\mathrm{line}}$. Nous présentons aussi des conditions suffisantes, en termes du domaine et des données au bord, pour que l'estimée logarithmique pour l'énergie soit satisfaite.

$\boxed{\text{Preprint.}}$

Chapter 2

Line defects in the vanishing elastic constant limit of a three-dimensional Landau-de Gennes model

Abstract

We consider the Landau-de Gennes variational model for nematic liquid crystals, in three-dimensional domains. We are interested in the asymptotic behaviour of minimizers as the elastic constant tends to zero. Assuming that the energy of minimizers blows up at most logarithmically, there exists a relatively closed, 1-rectifiable set $\mathscr{S}_{\mathrm{line}}$ of finite length, such that minimizers converge to a locally harmonic map away from $\mathscr{S}_{\mathrm{line}}$. We also provide some sufficient conditions for the logarithmic energy bound to be satisfied.

Contents

Keywords. Landau-de Gennes model, Q-tensors, asymptotic analysis, singularities, line defects, rectifiable sets.
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2.1 Introduction

2.1.1 Variational models for nematic liquid crystals

A nematic liquid crystal is matter in an intermediate state between liquid and crystalline solid. Molecules can flow as in a liquid, but they are oriented in an ordered way. As a result, the material is anisotropic with respect to optic and electromagnetic properties. Here, we restrict our attention to uniaxial nematics. These materials are composed by rod-shaped (sometimes, disk-shaped) molecules, with indistinguishable ends. The symmetry group of such a molecule is generated by rotations around the molecular axis, and the reflection symmetry which exchange the ends of the molecules. The word *nematic* was coined by Friedel, and originates from the line defects which are observed in these materials (see [49]):

> *I am going to use the term nematic (νῆμα, thread) to describe the forms, bodies, phases, etc. of the second type... because of the linear discontinuities, which are twisted like threads, and which are one of their most prominent characteristics.*

In addition to line defects, also called *disclinations*, nematic media exhibit "hedgehog-like" point singularities. According to the topological theory of ordered media (see [99]), both kinds of defects are described by the homotopy groups of a manifold, which parametrizes the possible local configurations of the material.

Three main continuum theories for uniaxial nematic liquid crystals have drawn the attention of the mathematical community: the Oseen-Frank, the Ericksen and the Landau-de Gennes theories. In the Oseen-Frank theory [48], the material is modeled by a unit vector field $\mathbf{n} = \mathbf{n}(x) \in \mathbb{S}^2$, which represents the preferred direction of molecular alignment. The elastic energy, in the simplest setting, reduces to the Dirichlet functional

$$E(\mathbf{n}) := \frac{1}{2}\int_\Omega |\nabla \mathbf{n}|^2\,, \tag{2.1.1}$$

where $\Omega \subseteq \mathbb{R}^3$ is the physical domain. In this case, least-energy configurations are but harmonic maps $\mathbf{n}\colon \Omega \to \mathbb{S}^2$. As such, minimizers have been widely studied in the literature (the reader is referred to e.g. [70] for a general review of this subject). Schoen and Uhlenbeck [125] proved that minimizers are smooth away from a discrete set of points singularities. Brezis, Coron and Lieb [23] investigated the precise shape of minimizers around a point defect x_0, and proved that

$$\mathbf{n}(x) \simeq \pm R\frac{x - x_0}{|x - x_0|} \qquad \text{for } |x - x_0| \ll 1, \tag{2.1.2}$$

where R is a rotation. These "hedgehog-like" point defects are associated with a non-trivial homotopy class of maps $\mathbf{n}\colon \partial B_r(x_0) \to \mathbb{S}^2$, i.e. a non-trivial element of $\pi_2(\mathbb{S}^2)$. Interesting results are also available for the full Oseen-Frank energy, which consists of various terms accounting for splay, twist and bend deformations. Hardt, Kinderlehrer and Lin [60] proved the existence of minimizers and partial regularity, i.e. regularity out of an exceptional set whose Hausdorff dimension is strictly less than 1. As for the local behaviour of minimizers around the defects, the picture is not as clear as for the Dirichlet energy (2.1.1), but at least the stability of "hedgehog-like" singularities such as (2.1.2) as been completely analyzed (see [78] and the references therein). However, the partial regularity result of [60] implies that the Oseen-Frank theory cannot account for line defects.

Ericksen theory is less restrictive, because it allows spatially varying orientational order. Indeed, the configurations are described by a pair $(s, \mathbf{n}) \in \mathbb{R} \times \mathbb{S}^2$, where $\mathbf{n}$ is the preferred direction of molecular alignment and the scalar s measures the degree of ordering. In this theory, defects are identified by the condition $s = 0$, which correspond to complete disordered states. However, Ericksen itself was aware that his theory excluded configurations which might have physical reality (see [44]), and presented it as a "kind of compromise" between physical intuition and mathematical simplicity. Indeed, the Ericksen theory — just as the Oseen-Frank theory — postulates that, at each point of the medium, there is at most one preferred direction of molecular orientation. Configurations for which such a preferred direction exists are called *uniaxial*, because they have one axis of rotational symmetry. If no preferred direction exists, the configuration is called *isotropic* (in the Ericksen theory, this corresponds to $s = 0$).

The Landau-de Gennes theory [38] allows for a rather complete description of the local behaviour of the medium, because it accounts for *biaxial*[1] configurations as well. A state is called biaxial when it has no axis of rotational symmetry, but three orthogonal axes of reflection symmetry instead. In a biaxial state, more preferred directions of molecular alignment coexist (see [108] for more details). What makes the Landau-de Gennes theory so rich is the choice of the order parameter space. Configurations are described by matrices (the so-called Q-tensors), which can be interpreted as renormalized second-order moments of a microscopic density, representing the distribution of molecules as a function of orientation.

In this chapter, we aim at describing the generation of line defects for nematics in three-dimensional domains from a variational point of view, within the Landau-de Gennes theory. Two main simplifying assumptions are postulated here. First, we neglect the effect of external electromagnetic fields. Instead, to induce non-trivial behaviour in minimizers, we couple the problem with non-homogeneous Dirichlet boundary conditions (strong anchoring). Second, we adopt the one-constant approximation, that is we drop out several terms in the expression of the elastic energy, and we are left with the gradient-squared term only. These assumptions, which drastically reduce the technicality of the problem, are common in the mathematical literature on this subject (see e.g. [41, 51, 71, 73, 83, 98]). For the two-dimensional case, the analysis of the analogous problem is presented in [29, 55].

2.1.2 The Landau-de Gennes functional

As we mentioned before, the local configurations of the medium are described by Q-tensors, i.e. elements of

$$\mathbf{S}_0 := \left\{ Q \in \mathrm{M}_3(\mathbb{R}) \colon Q^\mathsf{T} = Q, \ \operatorname{tr} Q = 0 \right\}.$$

This is a real linear space, of dimension five, which we endow with the scalar product $Q \cdot P := Q_{ij} P_{ij}$ (Einstein's convention is assumed). This choice of the configurations space can be justified as follows. At a microscopic scale, the distribution of molecules around a given point $x \in \Omega$, as a function of orientation, can be represented by a probability measure μ_x on the unit sphere $\mathbb{S}^2$. The measure μ_x satisfies to the condition $\mu_x(B) = \mu_x(-B)$ for all $B \in \mathscr{B}(\mathbb{S}^2)$, which accounts for the head-to-tail symmetry of the molecules. Then, the simplest meaningful way to condense the information conveyed by μ_x is to consider the second-order moment

$$Q = \int_{\mathbb{S}^2} \left(\mathbf{n}^{\otimes 2} - \frac{1}{3} \operatorname{Id} \right) \mathrm{d}\mu_x(\mathbf{n}).$$

This quantity is renormalized, so that the isotropic state $\mu_x = \mathscr{H}^2 \llcorner \mathbb{S}^2$ corresponds to $Q = 0$. As a result, Q is a symmetric traceless matrix. (The interested reader is referred e.g. to [108] for further details.)

The (simplified) Landau-de Gennes functional reads

$$E_\varepsilon(Q) := \int_\Omega \left\{ \frac{1}{2} |\nabla Q|^2 + \frac{1}{\varepsilon^2} f(Q) \right\}, \qquad (\mathrm{LG}_\varepsilon)$$

1. Here "uniaxial" and "biaxial" refer to *arrangements* of molecules, not to the molecules themselves which are always assumed to be uniaxial.

where $Q\colon \Omega \to \mathbf{S}_0$ is the configuration of the medium, located in a bounded container $\Omega \subseteq \mathbb{R}^3$. The function f is the quartic Landau-de Gennes potential, defined by

$$f(Q) = k - \frac{a}{2}\operatorname{tr} Q^2 - \frac{b}{3}\operatorname{tr} Q^3 + \frac{c}{4}\left(\operatorname{tr} Q^2\right)^2 \qquad \text{for } Q \in \mathbf{S}_0. \tag{2.1.3}$$

This expression for f has been derived by a formal expansion in powers of Q. All the terms are invariant by rotations so that f is independent of the coordinate frame. This potential allows for multiple local minima, with a first-order isotropic-nematic phase transition (see [38, 140]). The positive parameters a, b and c depend on the material and the temperature (which is assumed to be uniform and constant), whereas k is just an additive constant, which plays no role in the minimization problem. The potential f is bounded from below, so we determine uniquely the value of k by requiring $\inf f = 0$. The parameter ε^2 is a material-dependent elastic constant, typically very small ($\varepsilon^2 \simeq 10^{-11}$ Jm^{-1}, as order of magnitude). For each $0 < \varepsilon < 1$, we assign a boundary datum $g_\varepsilon \in H^1(\partial\Omega,\, \mathbf{S}_0)$ and we restrict our attention to minimizers Q_ε of (LG$_\varepsilon$) in the class

$$H^1_{g_\varepsilon}(\Omega,\, \mathbf{S}_0) := \left\{Q \in H^1(\Omega,\, \mathbf{S}_0)\colon Q_{|\partial\Omega} = g_{\varepsilon|\partial\Omega} \text{ in the sense of traces}\right\}.$$

The set $\mathscr{N} := f^{-1}(0)$ is involved in the analysis of the problem. Indeed, when ε is very small the term $\varepsilon^{-2} f(Q)$ in (LG$_\varepsilon$) forces minimizers to take their values as close as possible to $\mathscr{N}$. The set $\mathscr{N}$ can be characterized as follows (see [98, Proposition 9]):

$$\mathscr{N} = \left\{s_*\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\operatorname{Id}\right) : \mathbf{n} \in \mathbb{S}^2\right\}, \tag{2.1.4}$$

where the constant s_* is defined by

$$s_* = s_*(a,\, b,\, c) := \frac{1}{4c}\left(b + \sqrt{b^2 + 24ac}\right).$$

Thus, $\mathscr{N}$ is a smooth submanifold of $\mathbf{S}_0$, diffeomorphic to the real projective plane $\mathbb{RP}^2$, called *vacuum manifold*. The topology of $\mathscr{N}$ plays an important role, for a map $\Omega \to \mathscr{N}$ may encounter topological obstructions to regularity. Sources of obstruction are the homotopy groups $\pi_1(\mathscr{N}) \simeq \mathbb{Z}/2\mathbb{Z}$ and $\pi_2(\mathscr{N}) \simeq \mathbb{Z}$, which are associated with line and point singularities, respectively. There is a remarkable difference with the Oseen-Frank model at this level, for $\mathbb{S}^2$ is a simply connected manifold, so topological obstructions result from $\pi_2(\mathbb{S}^2)$ only. Despite this fact, a strong connection between the Oseen-Frank and Landau-de Gennes theories was established by Majumdar and Zarnescu. In their paper [98], they addressed the asymptotic analysis of minimizers of (LG$_\varepsilon$), in three-dimensional domains. Their results imply that, when Ω, $\partial\Omega$ are simply connected and $g_\varepsilon = g \in C^1(\partial\Omega,\, \mathscr{N})$, minimizers Q_ε of (LG$_\varepsilon$) converge in $H^1(\Omega,\, \mathbf{S}_0)$ to a map of the form

$$Q_0(x) = s_*\left(\mathbf{n}_0^{\otimes 2}(x) - \frac{1}{3}\operatorname{Id}\right)$$

where $\mathbf{n}_0 \in H^1(\Omega,\, \mathbb{S}^2)$ is a minimizer of (2.1.1). The convergence is locally uniform, away from singularities of Q_0. Also in this case, line defects do not appear in the limiting map, although point defects analogous to (2.1.2) might occur. Indeed, their assumptions on the domain and boundary datum are strong enough to guarantee the uniform energy bound

$$E_\varepsilon(Q_\varepsilon) \leq C \tag{2.1.5}$$

for an ε-independent constant C, and obtain H^1-compactness. In this chapter, we work in the logarithmic energy regime

$$E_\varepsilon(Q_\varepsilon) \leq C\left|\log\varepsilon\right|, \tag{2.1.6}$$

which is compatible with singularities of codimension two, in the ε-vanishing limit.

There are analogies between the functional (LG_ε) and the Ginzburg-Landau energy for superconductors, which reduces to

$$E_\varepsilon^{\mathrm{GL}}(u) := \int_\Omega \left\{ \frac{1}{2} |\nabla u|^2 + \frac{1}{4\varepsilon^2} \left(1 - |u|^2\right)^2 \right\} \tag{2.1.7}$$

when no external field is applied. Here the unknown is a complex-valued function u. There is a rich literature about the asymptotic behaviour, as $\varepsilon \to 0$, of critical points satisfying a logarithmic energy bound such as (2.1.6). It is well-known that, under appropriate assumptions, critical points converge to maps with topology-driven singularities of codimension two. In two-dimensional domains, the theory has been developed after Bethuel, Brezis and Hélein's work [14]. In the three-dimensional case, the asymptotic analysis of minimizers was performed by Lin and Rivière [89], and extended to non-minimizing critical points by Bethuel, Brezis and Orlandi [15]. Later, Jerrard and Soner [76] and Alberti, Baldo, Orlandi [2] proved independently that $|\log \varepsilon|^{-1} E_\varepsilon^{\mathrm{GL}}$ Γ-converges, when $\varepsilon \to 0$, to a functional on integral currents of codimension two. This functional essentially measures the length of defect lines, weighted by some quantity that accounts for the topology of the defect.

2.1.3 Main results

For each fixed $\varepsilon > 0$, a classical argument of Calculus of Variations shows that minimizers of (LG_ε) exist as soon as $g_\varepsilon \in H^{1/2}(\partial\Omega, \mathbf{S}_0)$. Our main result deals with their asymptotic behaviour as $\varepsilon \to 0$.

Theorem 2.1.1. *Let Ω be a bounded, Lipschitz domain. Assume that there exists a positive constant M such that, for any $0 < \varepsilon < 1$, there hold*

$$E_\varepsilon(Q_\varepsilon) \leq M\left(|\log \varepsilon| + 1\right) \qquad \text{and} \qquad \|Q_\varepsilon\|_{L^\infty(\Omega)} \leq M. \tag{H}$$

Then, there exist a subsequence $\varepsilon_n \searrow 0$, a relatively closed set $\mathscr{S}_{\mathrm{line}} \subseteq \Omega$ and a map $Q_0 \in H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathscr{N})$ such that the following holds.

(i) $\mathscr{S}_{\mathrm{line}}$ is a countably $\mathscr{H}^1$-rectifiable set, and $\mathscr{H}^1(\mathscr{S}_{\mathrm{line}}) < +\infty$.

(ii) For any open set $K \subset\subset \Omega$, either $\mathscr{S}_{\mathrm{line}} \cap K$ is empty or it has Hausdorff dimension equal to 1.

(iii) $Q_{\varepsilon_n} \to Q_0$ strongly in $H^1_{\mathrm{loc}}(\Omega \setminus \mathscr{S}_{\mathrm{line}}, \mathscr{N})$.

(iv) Q_0 is locally minimizing harmonic in $\Omega \setminus \mathscr{S}_{\mathrm{line}}$, that is for every ball $B \subset\subset \Omega \setminus \mathscr{S}_{\mathrm{line}}$ and any $P \in H^1(B, \mathscr{N})$, if $P_{|\partial B} = Q_{0|\partial B}$ then

$$\frac{1}{2}\int_B |\nabla Q_0|^2 \leq \frac{1}{2}\int_B |\nabla P|^2 .$$

(v) There exists a locally finite set $\mathscr{S}_{\mathrm{pts}} \subseteq \Omega \setminus \mathscr{S}_{\mathrm{line}}$ such that Q_0 is smooth on $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$ and $Q_\varepsilon \to Q_0$ locally uniformly in $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$.

By saying that $\mathscr{S}_{\mathrm{line}}$ is countably $\mathscr{H}^1$-rectifiable we mean that there exists a decomposition

$$\mathscr{S}_{\mathrm{line}} = \bigcup_{j \in \mathbb{N}} \mathscr{S}_j,$$

where $\mathscr{H}^1(\mathscr{S}_0) = 0$ and, for each $j \geq 1$, the set $\mathscr{S}_j$ is the image of a Lipschitz function $\mathbb{R} \to \mathbb{R}^3$. Roughly speaking, Condition (ii) means that $\mathscr{S}_{\mathrm{line}}$ contains no such things as Cantor-type components.

Theorem 2.1.1 is local in nature. In particular, boundary conditions play no particular role in the proof of this result, although they need to be imposed to induce non-trivial behaviour of minimizers. In addition to the singular set $\mathscr{S}_{\mathrm{line}}$, the limiting map Q_0 may have a set of point singularities $\mathscr{S}_{\mathrm{pts}}$. This is consistent with the regularity results for minimizing harmonic maps [53, 125]. As simple examples show, in general the regularity of Q_0 cannot be improved to obtain $\mathscr{S}_{\mathrm{pts}} = \emptyset$. For instance, one may take the unit ball as domain and impose the boundary condition $Q_{\varepsilon|\partial\Omega} = g_{|\partial\Omega}$, where

$$g(x) := s_* \left\{ \left(\frac{x}{|x|} \right)^{\otimes 2} - \frac{1}{3} \mathrm{Id} \right\} \qquad \text{for } x \in \mathbb{R}^3 \setminus \{0\}.$$

In this case, the results of [23, 98] imply the H^1-convergence $Q_\varepsilon \to g$ on the whole of the domain, so $\mathscr{S}_{\mathrm{line}} = \emptyset$ but $\mathscr{S}_{\mathrm{pts}} = \{0\}$. In this example, the singularity is induced by the homotopically non-trivial behaviour of the boundary datum. However, topological obstructions are not the only source of defects. When the dimension of the domain is three, point singularities of Q_0 may arise simply because it is energetically convenient to do so. This phenomenon has been remarked in the context of harmonic maps by Hardt and Lin [62]. Based on this fact, one expects that there exists minimizing configurations with line singularities, induced by topology, where at the same time point singularities appear for energetic reasons.

As for the properties of the singular set $\mathscr{S}_{\mathrm{line}}$, we also prove the

Proposition 2.1.2. *There exists a bounded, $\mathscr{H}^1$-integrable, Borel function $\Theta\colon \mathscr{S}_{\mathrm{line}} \to \mathbb{R}^+$ such that $\mathbf{V}(\mathscr{S}_{\mathrm{line}}, \Theta)$ is a stationary varifold.*

Here $\mathbf{V}(\mathscr{S}_{\mathrm{line}}, \Theta)$ is defined as the equivalence class of all pairs $(\mathscr{S}', \Theta')$, with $\mathscr{S}'$ being a countably $\mathscr{H}^1$-rectifiable set, $\mathscr{H}^1((\mathscr{S} \setminus \mathscr{S}') \cup (\mathscr{S}' \setminus \mathscr{S})) = 0$, and $\Theta = \Theta'$ $\mathscr{H}^1$-a.e. on $\mathscr{S} \cap \mathscr{S}'$. The definition of stationary varifold is given in [131, Chapter 4]. Varifolds are a generalization of differentiable manifolds, introduced by Almgren [4] in the context of Calulus of Variations. Stationary varifolds can be though as a weak notion of manifolds with vanishing mean curvature. Unfortunately, very few regularity results are known for general stationary varifolds. In Proposition 2.1.2, both the set $\mathscr{S}_{\mathrm{line}}$ and the density Θ are obtained from the energy density of minimizers Q_ε, passing to the limit as $\varepsilon \to 0$ in a weak sense.

We provide sufficient conditions for the estimates (H) to hold, in terms of the domain and the boundary data. Here is our first condition.

(H_1) Ω is a bounded, smooth domain and $\{g_\varepsilon\}_{0<\varepsilon<1}$ is a bounded family in $H^{1/2}(\partial\Omega, \mathscr{N})$.

The uniform $H^{1/2}$-bound is satisfied if, for instance, $g_\varepsilon = g\colon \partial\Omega \to \mathscr{N}$ has a finite number of disclinations. This means, there exists a finite set $\Sigma \subseteq \partial\Omega$ such that g is smooth on $\partial\Omega \setminus \Sigma$ and around each $x_0 \in \Sigma$ the map g can be written as

$$g(\rho, \theta) = s_* \left\{ \left(\tau_1 \cos\frac{\theta}{2} + \tau_2 \sin\frac{\theta}{2} \right)^{\otimes 2} - \frac{1}{3} \mathrm{Id} \right\} + \text{smooth terms of order } \rho \qquad \text{as } \rho \to 0, \tag{2.1.8}$$

where (ρ, θ) are geodesic polar coordinates centered at x_0 and (τ_1, τ_2) is an orthonormal pair in $\mathbb{R}^3$.

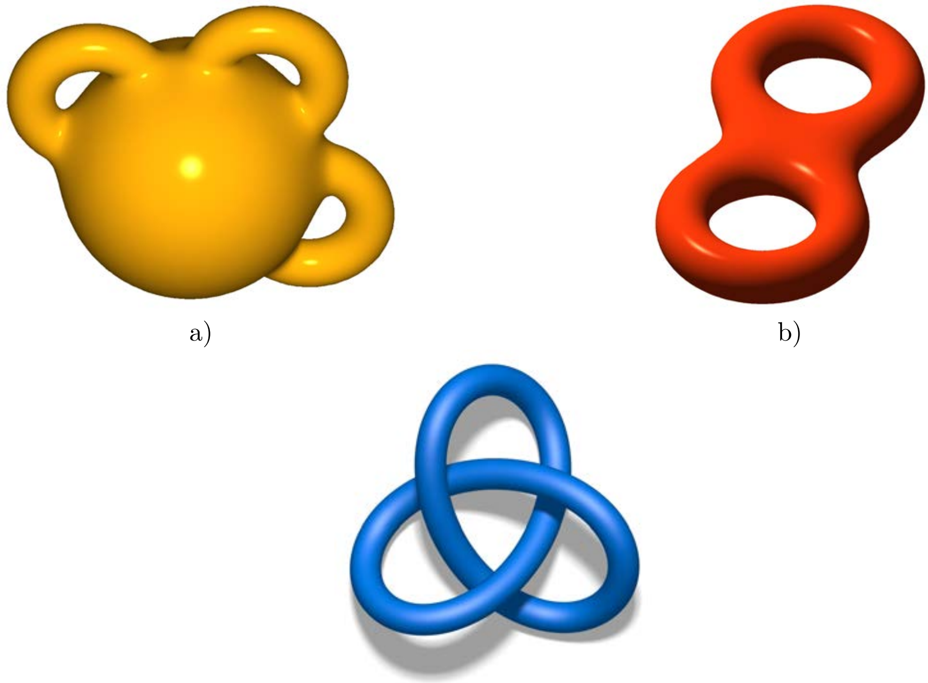
Proposition 2.1.3. *Condition* (H_1) *implies* (H).

Alternatively, one can assume

(H_2) $\Omega \subseteq \mathbb{R}^3$ is a bounded Lipschitz domain, and it is bilipschitz equivalent to a handlebody (i.e. a 3-ball with a finite number of handles attached).

(H_3) There exists $M_0 > 0$ such that, for any $0 < \varepsilon < 1$, we have $g_\varepsilon \in (H^1 \cap L^\infty)(\partial\Omega, \mathbf{S}_0)$ and

$$E_\varepsilon(g_\varepsilon, \partial\Omega) \leq M_0 \left(|\log \varepsilon| + 1 \right), \qquad \|g_\varepsilon\|_{L^\infty(\partial\Omega)} \leq M_0.$$



a) b)

c)

Figure 2.1: a) sphere with three handles; b) a torus with two holes; c) a tubular neighborhood of a trefoil knot. The domains in a) and b) satisfy Condition (H_2). Notice that every domain satisfying (H_2) has a connected boundary, but the converse is not true. For instance, if K is the set shown in c), then the 1-point compactification of $\mathbb{R}^3 \setminus K$ is a domain with connected boundary, which does *not* satisfy (H_2).

As an example of sequence satisfying (H_3), one can take smooth approximations of a map $g\colon \partial\Omega \to \mathscr{N}$ of the form (2.1.8). For instance, we might take

$$g_\varepsilon(\rho,\, \theta) := \eta_\varepsilon(\rho) g(\rho,\, \theta) \tag{2.1.9}$$

where $\eta_\varepsilon \in C^\infty[0,\, +\infty)$ is such that

$$\eta_\varepsilon(0) = \eta_\varepsilon'(0) = 0, \qquad \eta_\varepsilon(\rho) = 1 \text{ si } \rho \geq \varepsilon, \qquad 0 \leq \eta_\varepsilon \leq 1, \qquad |\eta_\varepsilon'| \leq C\varepsilon^{-1}.$$

Proposition 2.1.4. *Assumptions* (H_2) *and* (H_3) *imply* (H).

Remark 2.1.1. Hypothesis (H_2) is *not* the same as asking Ω to be a bounded Lipschitz domain with connected boundary. Let $K \subseteq \mathbb{S}^3$ be a (closed) tubular neighborhood of a trefoil knot. Then K is a solid torus, i.e. K is diffeomorphic to $\mathbb{S}^1 \times B^2_1$, but $\mathbb{S}^3 \setminus K$ is *not* a solid torus. In fact, $\mathbb{S}^3 \setminus K$ is not even a handlebody, because

$$\pi_1(\mathbb{S}^2 \setminus K) = \text{ the knot group of the trefoil knot } = \left\langle x,\, y \,|\, x^2 = y^3 \right\rangle$$

whereas the fundamental group of any handlebody is free. By composing with a stereographic projection, one constructs a smooth domain $\Omega \subseteq \mathbb{R}^3$ diffeomorphic to $\mathbb{S}^3 \setminus K$. In particular, $\partial\Omega$ is a torus but Ω does not satisfies (H_2).

We can give examples where the limit map Q_0 has a line defect. In fact, given *any* bounded smooth domain, one can find a family of boundary data such that the energy of minimizers blows up as $\varepsilon \to 0$.

Proposition 2.1.5. *For each bounded domain $\Omega \subseteq \mathbb{R}^3$ of class C^1, there exists a family of boundary data $\{g_\varepsilon\}_{0<\varepsilon<1}$ satisfying* (H_3) *and a number $\alpha > 0$ such that*

$$E_\varepsilon(Q) \geq \alpha \left(|\log \varepsilon| - 1 \right)$$

for any $Q \in H^1_{g_\varepsilon}(\Omega, \mathbf{S}_0)$ *and any* $0 < \varepsilon < 1$*. In particular, there is no subsequence of minimizers which converges in* $H^1(\Omega, \mathbf{S}_0)$*.*

The functions g_ε are constructed as smooth approximations of a map $\partial\Omega \to \mathscr{N}$ with point singularities, as in (2.1.9). In this case, the corresponding set $\mathscr{S}_{\mathrm{line}}$ is non-empty (although it may lie on the boundary of Ω — se Remark 2.5.1).

Let us spend a few word on the proof of our main result, Theorem 2.1.1. The core of the argument is a concentration property for the energy, which can be stated as follows.

Proposition 2.1.6. *Assume that the condition* (H) *holds. For any* $0 < \theta < 1$ *there exist positive numbers* η*,* ϵ_0 *and* C *such that, for any* $x_0 \in \Omega$*,* $R > 0$ *satisfying* $B_R(x_0) \subset\subset \Omega$ *and any* $0 < \varepsilon \leq \epsilon_0 R$*, if*

$$E_\varepsilon(Q_\varepsilon, B_R(x_0)) \leq \eta R \log \frac{R}{\varepsilon} \tag{2.1.10}$$

then

$$E_\varepsilon(Q_\varepsilon, B_{\theta R}(x_0)) \leq CR.$$

Proposition 2.1.6 implies that either the energy on a ball blows up at least logarithmically, or it is bounded on a smaller ball. Combining this fact with covering arguments, one proves that the energy concentrates on a set $\mathscr{S}_{\mathrm{line}}$ of finite $\mathscr{H}^1$-measure. Then, the asymptotic behaviour of minimizers away from $\mathscr{S}_{\mathrm{line}}$ can be studied using well-established techniques, e.g. arguing as in [98].

Roughly speaking, the proof of Proposition 2.1.6 goes as follows. Close to a topological singularity of codimension two, the energy is of the order of $\kappa_*|\log\varepsilon|$ for a positive constant κ_*, by Jerrard-Sandier type estimates (see [75, 123]). Therefore, if η is small compared to κ_*, Condition (2.1.10) implies that the sphere $\partial B_r(x_0)$ intersects no topological defect line of Q_ε, for a sufficiently large subset of radii $r \in (\theta R, R)$. Because there is no topological obstruction, one can approximate Q_ε with a $\mathscr{N}$-valued map P_ε defined on the sphere $\partial B_r(x_0)$. By adapting Luckhaus' construction [92, Lemma 1], one defines a map φ_ε on a thin spherical shell $B_r(x_0) \setminus B_{r'}(x_0)$, such that $\varphi_\varepsilon = Q_\varepsilon$ on $\partial B_r(x_0)$ and $\varphi_\varepsilon = P_\varepsilon$ on $\partial B_{r'}(x_0)$. Since $\partial B_{r'}(x_0)$ is simply connected, P_ε can be lifted to a $\mathbb{S}^2$-valued map, i.e. one can write

$$P_\varepsilon(x) = s_*\left(\mathbf{n}_\varepsilon^{\otimes 2}(x) - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{for } x \in \partial B_{r'}(x_0)$$

for a smooth map $\mathbf{n}_\varepsilon \colon \partial B_{r'}(x_0) \to \mathbb{S}^2$. This is a crucial point in the proof, for it makes possible to apply the methods by Hardt, Kinderlehrer and Lin [60, Lemma 2.3] and obtain boundedness for the energy, via a comparison argument. In other words, on simply connected regions where no obstruction occurs from $\pi_1(\mathscr{N})$, the asymptotic analysis of the Landau-de Gennes problem can be reduced to the analysis of the Oseen-Frank problem, by lifting. Extension results are needed in several steps of this proof, for instance to construct the interpolation map φ_ε. Various results in this direction are discussed in detail in Section 2.3. In particular, we prove variants of Luckhaus' lemma [92, Lemma 1] which are fit for our purposes.

Remark 2.1.2. By Theorem 2.1.1, Condition (H) yields compactness for the sequence [2] $\{Q_\varepsilon\}_{0<\varepsilon<1}$. An analogous property does *not* hold for the Ginzburg-Landau energy (2.1.7). Indeed, a counter-example by Brezis and Mironescu [24] shows that there exist minimizers $u_\varepsilon \in H^1(B_1^2, \mathbb{C})$ such that

$$E_\varepsilon^{\mathrm{GL}}(u_\varepsilon, B_1^2) \ll |\log\varepsilon| \qquad \text{and} \qquad |u_\varepsilon| \leq 1,$$

yet $\{u_\varepsilon\}_{0<\varepsilon<1}$ does not have subsequences converging a.e. on sets of positive measure. The boundary data $g_\varepsilon := u_{\varepsilon|\partial B_1^2}$ are highly-oscillating $\mathbb{S}^1$-valued maps. In particular, the g_ε's can be lifted to $\mathbb{R}$-valued functions φ_ε (that is $g_\varepsilon = \exp(i\varphi_\varepsilon)$), but (φ_ε) *is not a bounded sequence.* This phenomenon cannot occur in our case, because $\mathscr{N}$-valued maps are lifted to $\mathbb{S}^2$-valued maps, so the lifting sequence takes values in a compact manifold. Therefore, finiteness of the fundamental group $\pi_1(\mathscr{N})$ yields better compactness properties for minimizers.

2. Throughout the chapter, the word "sequence" will be used to denote family of functions indexed by a continuous parameter as well.

2.1.4 Concluding remarks and open questions

Several questions about minimizers of the Landau-de Gennes functional on three-dimensional domains remain open. A first question concerns the structure of the singular set $\mathscr{S}_{\mathrm{line}}$. Since $\mathscr{S}_{\mathrm{line}}$ is obtained by taking the limit of a sequence of minimizers, one would expect that it inherits from Q_ε minimizing properties, such as being a set of minimal length. If the domain is convex and the boundary data has a finite number of point singularities $x_1, \ldots, x_p$ of the form (2.1.8), it is natural to conjecture that $\mathscr{S}_{\mathrm{line}}$ is a union of non-intersecting straight lines connecting the x_i's in pairs. (Note that, by topological arguments, the number p must be even.)

It would be interesting to study the behaviour of minimizers Q_ε in a small tube around $\mathscr{S}_{\mathrm{line}}$. In particular, one could ask whether there are isotropic ($Q(x) = 0$) or biaxial points (the eigenvalues of $Q(x)$ are all different from each other) in the core of defects. Contreras and Lamy [35] proved that the core of point singularities, in dimension three, contains biaxial phases when the temperature is low enough, but their proof uses a uniform energy bound such as (2.1.5) so it does not apply to singularities of codimension two. However, the analysis of point defects on two-dimensional domains (see e.g. [29, 41]) might indicate that line defects also contain biaxial phases, when the temperature is low.

In another direction, investigating the asymptotic behaviour of a more general class of functionals in the logarithmic energy regime is a challenging issue. For instance, one may consider functionals with more elastic energy terms and/or choose different potentials, such as the sextic potential

$$f(Q) := -\frac{a_1}{2}\operatorname{tr} Q^2 - \frac{a_2}{3}\operatorname{tr} Q^3 + \frac{a_3}{4}\left(\operatorname{tr} Q^2\right)^2 + \frac{a_4}{5}\left(\operatorname{tr} Q^2\right)\left(\operatorname{tr} Q^3\right) + \frac{a_5}{6}\left(\operatorname{tr} Q^2\right)^3 + \frac{a_5'}{6}\left(\operatorname{tr} Q^3\right)^2$$

(see [36, 58]) or the singular potential proposed by Ball and Majumdar [9]. Dealing with the Landau-de Gennes functional in full generality will probably require new techniques, but hopefully the variational arguments presented here could be of help to the study of simple cases.

The chapter is organized as follows. Section 2.2 deals with general facts about the space of Q-tensors and Landau-de Gennes minimizers. In particular, lower estimates for the energy of maps $B^2_1 \to \mathbf{S}_0$ are established in Subsection 2.2.2, by adapting Jerrard's and Sandier's arguments. Section 2.3 deals with extension problems. The results of this section are a fundamental tool for the proof of the main results. Section 2.4 aims at proving Theorem 2.1.1. Proposition 2.1.6 is proved in Subsection 2.4.1. The asymptotic analysis away from the singular lines is carried out in Subsection 2.4.2, whereas the singular set $\mathscr{S}$ is defined and studied in Subsection 2.4.3. Section 2.5 deals with the proofs of Propositions 2.1.4 and 2.1.5.

2.2 Preliminary results

2.2.1 Properties of $\mathbf{S}_0$ and f

We discuss general facts about Q-tensors, which are useful in order to to have an insight into the structure of the target space $\mathbf{S}_0$. The starting point of our analysis is the following representation formula.

Lemma 2.2.1. *For all fixed $Q \in \mathbf{S}_0 \setminus \{0\}$, there exist two numbers $s \in (0, +\infty)$, $r \in [0, 1]$ and an orthonormal pair of vectors $(\mathbf{n}, \mathbf{m})$ in $\mathbb{R}^3$ such that*

$$Q = s\left\{\mathbf{n}^{\otimes 2} - \frac{1}{3}\operatorname{Id} + r\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\operatorname{Id}\right)\right\}.$$

Given Q, the parameters $s = s(Q)$, $r = r(Q)$ are uniquely determined. The functions $Q \mapsto s(Q)$ and $Q \mapsto r(Q)$ are continuous on $\mathbf{S}_0 \setminus \{0\}$, and are positively homogeneous of degree 1 and 0, respectively.

Slightly different forms of this formula are often found in the literature (e.g. [98, Proposition 1]). The proof is a straightforward computation sketched in Chapter 1 (Lemma 1.3.1), so we omit it here.

Remark 2.2.1. All the same, we would like to recall some properties of s, r (again, see Chapter 1 for a proof). The parameters $s(Q)$, $r(Q)$ are determined by the eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3$ of Q according to this formula:

$$s(Q) = 2\lambda_1 + \lambda_2, \qquad r(Q) = \frac{\lambda_1 + 2\lambda_2}{2\lambda_1 + \lambda_2}. \tag{2.2.1}$$

The functions s, r are positively homogeneous of degree one, zero respectively. Following [98, Proposition 15], the vacuum manifold $\mathscr{N} := f^{-1}(0)$ can be characterized as follows:

$$\mathscr{N} = \{Q \in \mathbf{S}_0 \colon s(Q) = s_*,\, r(Q) = 0\},$$

where

$$s_* := \frac{1}{4c}\left(b + \sqrt{b^2 + 24ac}\right).$$

In Chapter 1, we have considered another important subset of $\mathbf{S}_0$, namely

$$\mathscr{C} := \left\{Q \in \mathbf{S}_0 \setminus \{0\} \colon r(Q) = 1\right\} \cup \{0\}.$$

This is a closed subset of $\mathscr{C}$, and it is cone (that is, $\lambda Q \in \mathscr{C}$ whenever $Q \in \mathscr{C}$ and $\lambda \in \mathbb{R}^+$). Thanks to (2.2.1), we have

$$\mathscr{C} = \left\{Q \in \mathbf{S}_0 \colon \lambda_1(Q) = \lambda_2(Q)\right\},$$

so $\mathscr{C}$ is the set of matrices whose leading eigenvalue has multiplicity 2 or 3. As we have shown in the previous chapter, this set is relevant in understanding the topological structure of $\mathbf{S}_0$. We summarize the main properties of $\mathscr{C}$ in the following lemma.

Lemma 2.2.2. *The set $\mathscr{C} \setminus \{0\}$ is a smooth submanifold of $\mathbf{S}_0$ diffeomorphic to $\mathbb{RP}^2 \times \mathbb{R}$. The set $\mathbf{S}_0 \setminus \mathscr{C}$ retracts by deformation onto $\mathscr{N}$; a C^1-retraction is defined by the formula*

$$\mathscr{R}(Q) := s_*\left(\mathbf{n}^{\otimes 2}(Q) - \frac{1}{3}\operatorname{Id}\right) \qquad \text{for } Q \in \mathbf{S}_0 \setminus \mathscr{C},$$

where $\mathbf{n}(Q)$ is a unit eigenvector associated with $\lambda_1(Q)$. Moreover, $\mathscr{R}$ coincides with the nearest-point projection onto $\mathscr{N}$, that is

$$|Q - \mathscr{R}(Q)| \leq |Q - P| \tag{2.2.2}$$

holds for any $Q \in \mathbf{S}_0 \setminus \mathscr{C}$ and any $P \in \mathscr{N}$, with strict inequality if $P \neq \mathscr{R}(Q)$.

Proof. The regularity of $\mathscr{C} \setminus \{0\}$ and of $\mathscr{R}$, as well as the retraction property, have been proved in Chapter 1 (Lemmas 1.3.5–1.3.7), so we only need to show that $\mathscr{R}$ is the nearest point projection onto $\mathscr{N}$. To this end, we pick an arbitrary $Q \in \mathbf{S}_0 \setminus \mathscr{C}$ and $P \in \mathscr{N}$. By applying Lemma 2.2.1, we write

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\operatorname{Id}\right) + sr\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\operatorname{Id}\right) \qquad \text{and} \qquad P = s_*\left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\operatorname{Id}\right)$$

for some numbers $s > 0$ and $0 \leq r < 1$, some orthonormal pair $(\mathbf{n}, \mathbf{m})$ and some unit vector $\mathbf{p}$. We compute that

$$|Q - P|^2 = \frac{2}{3}s^2\left(r^2 - r + 1\right) + \frac{2}{3}s_* s(1 - r) + \frac{2}{3}s_*^2 - 2s_* s\left\{(\mathbf{n}\cdot\mathbf{p})^2 + r(\mathbf{m}\cdot\mathbf{p})^2\right\}.$$

Given s, r, $\mathbf{n}$ and $\mathbf{m}$, we minimize with respect to $\mathbf{p}$ the right-hand side, subject to the constraint

$$(\mathbf{n}\cdot\mathbf{p})^2 + (\mathbf{m}\cdot\mathbf{p})^2 \leq 1.$$

One easily sees that, since $r < 1$, the minimum is achieved if and only if $\mathbf{p} = \pm\mathbf{n}$, that is $P = \mathscr{R}(Q)$. $\square$

Given a bounded domain $U \subseteq \mathbb{R}^k$, a non-trivial boundary datum $g \in C^0(\partial U, \mathscr{N})$ and a map $Q \in C^0_g(U, \mathbf{S}_0)$, Lemma 2.2.2 implies that $Q^{-1}(\mathscr{C}) \neq \emptyset$. For otherwise $\mathscr{R} \circ Q \colon \Omega \to \mathscr{N}$ would be a well-defined, continuous extension of the boundary datum, which is a contradiction. In this sense, the condition $Q \in \mathscr{C}$ identify the regions where topological defect occurs.

We introduce another function, which is involved in the analysis of Subsection 2.2.2.

Lemma 2.2.3. *The function $\phi \colon \mathbf{S}_0 \to \mathbb{R}$ given by $\phi(0) = 0$,*

$$\phi(Q) := s_*^{-1} s(Q)(1 - r(Q)) \qquad \text{for } Q \in \mathbf{S}_0 \setminus \{0\}$$

is Lipschitz continuous on $\mathbf{S}_0$, of class C^1 on $\mathbf{S}_0 \setminus \mathscr{C}$ and satisfies

$$\sqrt{2} s_*^{-1} \leq |\mathrm{D}\phi(Q)| \leq 2 s_*^{-1} \qquad \text{for any } Q \in \mathbf{S}_0 \setminus \mathscr{C}.$$

Moreover, $\phi(Q) = 0$ if and only if $Q \in \mathscr{C}$.

Proof. By definition, it is clear that $\phi(Q) = 0$ if and only if $Q = 0$ or $r(Q) = 1$, that is $Q \in \mathscr{C}$. Using (2.2.1), we can write

$$s_* \phi(Q) = \lambda_1 - \lambda_2, \tag{2.2.3}$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3$ are the eigenvalues of Q. Thanks to standard regularity results for the eigenvalues (see e.g. [8, Equation (9.1.32) p. 598]), we immediately deduce that ϕ is locally Lipschitz continuous and of class C^1 on $\mathbf{S}_0 \setminus \mathscr{C}$. Let $(\mathbf{n}, \mathbf{m}, \mathbf{p})$ be an orthonormal set of eigenvectors relative to $(\lambda_1, \lambda_2, \lambda_3)$ respectively. Then, for any $Q \in \mathbf{S}_0 \setminus \mathscr{C}$ there holds

$$s_* |\mathrm{D}\phi(Q)| = \max_{B \in \mathbf{S}_0, \ |B| = 1} \left| \frac{\partial \phi}{\partial B}(Q) \right| = \max_{B \in \mathbf{S}_0, \ |B| = 1} |\mathbf{n} \cdot B\mathbf{n} - \mathbf{m} \cdot B\mathbf{m}|$$

(the last identity follows by differentiating (2.2.3), with the help of [8] again). This implies $|\mathrm{D}\phi(Q)| \leq 2$. Now, set

$$B_0 := \frac{1}{\sqrt{2}} \left(\mathbf{n}^{\otimes 2} - \mathbf{m}^{\otimes 2} \right) \in \mathbf{S}_0.$$

Since that $|\mathbf{n}^{\otimes 2}| = |\mathbf{m}^{\otimes 2}| = 1$ and $\mathbf{n}^{\otimes 2} \cdot \mathbf{m}^{\otimes 2} = 0$, it is straightforward to check that $|B_0| = 1$, so

$$s_* |\mathrm{D}\phi(Q)| \geq |\mathbf{n} \cdot B_0 \mathbf{n} - \mathbf{m} \cdot B_0 \mathbf{m}| = \frac{1}{\sqrt{2}} \left(|\mathbf{n}|^2 + |\mathbf{m}|^2 \right) = \sqrt{2}. \qquad \square$$

We conclude our discussion on the structure of the target space $\mathbf{S}_0$ by proving a couple of properties of the potential f, which will turn out to be useful.

Lemma 2.2.4. *The Landau-de Gennes potential f, defined by (2.1.3), enjoys the following properties. For any bounded set $\omega \subset\subset \mathbf{S}_0$, there exists a constant $\gamma_1 = \gamma_1(a, b, c, \omega) > 0$ such that*

$$f(Q) \geq \gamma_1 (1 - \phi(Q))^2 \qquad \text{for any } Q \in \omega. \tag{F$_1$}$$

Moreover, there exist $\gamma_2, \gamma_3, \delta_0 > 0$ such that, if $Q \in \mathbf{S}_0$ satisfies $\operatorname{dist}(Q, \mathscr{N}) \leq \delta_0$, then

$$f(Q) \geq \gamma_2 \operatorname{dist}^2(Q, \mathscr{N}) \tag{F$_2$}$$

and

$$f\left(tQ + (1-t)\pi(Q)\right) \leq \gamma_3 t^2 f(Q) \tag{F$_3$}$$

for every $0 \leq t \leq 1$.

Proof of (F_1). Using the representation formula of Lemma 2.2.1, we can compute $\operatorname{tr} Q^2$ and $\operatorname{tr} Q^3$ as functions of $s := s(Q)$, $t := s(Q)r(Q)$. This yields

$$f(Q) = k - \frac{a}{3}\left(s^2 - st + t^2\right) - \frac{b}{27}\left(2s^3 - 3s^2 t + 3s^2 t - 2t^3\right) + \frac{c}{9}\left(s^2 - st + t^2\right)^2 =: \tilde{f}(s,\, t).$$

We know that $(s_*,\, 0)$ is a minimizer for $\tilde{f}$ (see e.g. [98, Proposition 15]), so $\mathrm{D}^2\tilde{f}(s_*,\, 0) \geq 0$. Moreover, it is straightforward to compute that

$$\det \mathrm{D}^2\tilde{f}(s_*,\, 0) > 0$$

thus $\mathrm{D}^2\tilde{f}(s_*,\, 0) > 0$. As a consequence, there exist two numbers $\delta > 0$ and $C > 0$ such that

$$\tilde{f}(s,\, sr) \geq C(s_* - s)^2 + Cs^2r^2 \qquad \text{if } (s - s_*)^2 + s^2r^2 \leq \delta. \tag{2.2.4}$$

On the other hand, for each bounded set $\omega \subset\subset \mathbf{S}_0$ there exists a constant $M = M(\omega)$ such that $(s(Q) - s_*)^2 + s^2(Q)r^2(Q) \leq M$ for all $Q \in \omega$. By compactness, there exists also a constant $C' > 0$ such that

$$\tilde{f}(s,\, sr) \geq C' \qquad \text{if } \delta < (s - s_*)^2 + s^2r^2 \leq M. \tag{2.2.5}$$

Combining (2.2.4) and (2.2.5), and modifying the value of C if necessary, for any $Q \in \omega$, $s = s(Q)$, $r = r(Q)$ we obtain:

$$\tilde{f}(s,\, sr) \geq C(s_* - s)^2 + Cs^2r^2 \geq \frac{Cs_*^2}{2}\left(1 - \frac{s}{s_*} + \frac{sr}{s_*}\right)^2 = \frac{Cs_*^2}{2}\left(1 - \phi(Q)\right)^2. \qquad \square$$

Proof of (F_2)–(F_3). Since the group SO(3) acts transitively on the manifold $\mathscr{N}$ and the potential f is preserved by the action, it suffices to check (F_2)–(F_3) in a neighborhood of a point $Q_0 \in \mathscr{N}$. Indeed, for any $Q \in \mathbf{S}_0$ there exists $\mathbf{n} \in \mathbb{S}^2$ such that

$$\mathscr{R}(Q) = s_*\left(\mathbf{n}\mathbf{n}^\mathsf{T} - \frac{1}{3}\,\mathrm{Id}\right),$$

and there exists a matrix $R \in \mathrm{SO}(3)$ such that $R\mathbf{n} = \mathbf{e}_3$. As is easily checked, the function $\xi_R\colon Q \mapsto RQR^\mathsf{T}$ maps isometrically $\mathbf{S}_0$ onto itself. Then, (2.2.2) implies that ξ_R commutes with $\mathscr{R}$, so

$$\mathscr{R}(\xi_R(Q)) = \xi_R(\mathscr{R}(Q)) = s_*\left(R\mathbf{n}(R\mathbf{n})^\mathsf{T} - \frac{1}{3}\,\mathrm{Id}\right) = s_*\left(\mathbf{e}_3\mathbf{e}_3^\mathsf{T} - \frac{1}{3}\,\mathrm{Id}\right) =: Q_0.$$

On the other hand, f is invariant by composition with ξ_R (i.e. $f \circ \xi_R = f$) because it is a function of the scalar invariants of Q. Therefore, if (F_2)–(F_3) are satisfied in case $\mathscr{R}(Q) = Q_0$, then (F_2)–(F_3) are satisfied for all $Q \in \mathbf{S}_0$ by the same constants γ_2, γ_3, δ_0. Hence, we assume without loss of generality that $\mathscr{R}(Q) = Q_0$.

Any matrix $P \in \mathbf{S}_0$ can be written in the form

$$P = \begin{pmatrix} -\frac{1}{3}(s_* + x_0) + x_4 & x_3 & x_1 \\ x_3 & -\frac{1}{3}(s_* + x_0) - x_4 & x_2 \\ x_1 & x_2 & \frac{2}{3}(s_* + x_0) \end{pmatrix}$$

for some $x = (x_0,\, x_1,\, \ldots x_4) \in \mathbb{R}^5$. In Lemma 1.3.8,it is shown that $P - Q_0 \in T_{Q_0}\mathscr{N}$ if and only if $x_0 = x_3 = x_4 = 0$, and $P - Q_0$ is orthogonal to $T_{Q_0}\mathscr{N}$ if and only if $x_1 = x_2 = 0$. One can write f as a function of x and compute the second derivatives. The computations are straightforward, so we omit them here. One obtains that the hessian matrix $\mathrm{D}^2 f(Q_0)$ is diagonal, with

$$\frac{\partial^2 f}{\partial x_0^2}(Q_0) > 0, \qquad \frac{\partial^2 f}{\partial x_1^2}(Q_0) = \frac{\partial^2 f}{\partial x_2^2}(Q_0) = 0, \qquad \frac{\partial^2 f}{\partial x_3^2}(Q_0) = \frac{\partial^2 f}{\partial x_4^2}(Q_0) > 0.$$

Therefore,

$$0 < \alpha_1 := \min_\nu \frac{1}{2} D^2 f(Q_0)\nu\cdot\nu \leq \alpha_2 := \max_\nu \frac{1}{2} D^2 f(Q_0)\nu\cdot\nu < +\infty.$$

where the minimum and maximum are taken over all $\nu \perp T_{Q_0}\mathscr{N}$ with $|\nu| = 1$. Now, take $P = Q$ with $\mathscr{R}(Q) = Q_0$, fix $0 \leq t \leq 1$ and write the Taylor expansion of f around Q_0. The point Q_0 is a minimizer for f, so $\mathrm{D}f(Q_0) = 0$ and

$$f(Q_0 + t(Q - Q_0)) = \frac{t^2}{2}\mathrm{D}^2 f(Q_0)(Q - Q_0)\cdot(Q - Q_0) + \mathrm{o}\left(t^2(Q - Q_0)^2\right)$$

In particular, if $|Q - Q_0| \leq \delta_0$ and δ_0 is small enough, then

$$\frac{1}{2}\alpha_1 t^2 |Q - Q_0|^2 \leq f(Q_0 + t(Q - Q_0)) \leq 2\alpha_2 t^2 |Q - Q_0|^2 .$$

The inequality (F$_2$) follows by taking $t = 1$ and setting $\gamma_2 := \alpha_1/2$. As for (F$_3$), combining this upper bound with (F$_2$) we obtain

$$f(Q_0 + t(Q - Q_0)) \leq 2\gamma_2^{-1}\alpha_2 t^2 f(Q),$$

so (F$_3$) is proved for $\gamma_3 := 2\gamma_2^{-1}\alpha_2$. □

2.2.2 Energy estimates in 2-dimensional domains

Throughout the chapter, we will use the following notation. For any $Q \in H^1(\Omega, \mathbf{S}_0)$ and any k-submanifold $U \subseteq \Omega$, we set

$$e_\varepsilon(Q) := \frac{1}{2}|\nabla Q|^2 + \frac{1}{\varepsilon^2} f(Q), \qquad E_\varepsilon(Q, U) := \int_U e_\varepsilon(Q)\,\mathrm{d}\mathscr{H}^k.$$

The function $e_\varepsilon(Q)$ is the energy density of Q.

The aim of this subsection is to prove a lower bound for the energy of maps $B^2_1 \to \mathbf{S}_0$, inspired by the fundamental estimates by Jerrard [75] and Sandier [123].

Proposition 2.2.5. *There exists a number κ_*, depending only on f, with the following property. Let $0 < \varepsilon < R$, $K > 0$ and let $Q \in W^{1,\infty}(B^2_R, \mathbf{S}_0)$ be any map satisfying*

$$\|Q\|_{L^\infty(B^2_R)} + \varepsilon\|\nabla Q\|_{L^\infty(B^2_R)} \leq K \tag{2.2.6}$$

and

$$Q(x) \notin \mathscr{C} \quad \text{for all } x \in B^2_R \setminus B^2_{R/2}. \tag{2.2.7}$$

If the homotopy class of $\mathscr{R}(Q_{|\partial B^2_R})$ is non-trivial, then

$$E_\varepsilon(Q, B^2_R) \geq \kappa_* \log\frac{R}{\varepsilon} - C,$$

where C is a constant depending only on K.

The energetic cost associated with topological defects is quantified by a number κ_*, defined by (2.2.15) and explicitely computed in Lemma 2.2.9:

$$\kappa_* = \frac{\pi}{2}s_*^2.$$

This number plays the same role as the quantity $\pi|\deg(u, \partial B^2_R)|$, which appears in Jerrard-Sandier type estimates for maps $u\colon B^2_R \to \mathbb{S}^1$. Proposition 2.2.5 is based on Jerrard's statement, but variants which are closer to Sandier's results can also be proved (see, e.g., Lemma 1.4.13). Before dealing with the proof of Proposition 2.2.5, we state an immediate consequence.

Corollary 2.2.6. *Assume that $Q \in W^{1,\infty}(B^2_R, \mathbf{S}_0)$ satisfies (2.2.6), for some $0 < \varepsilon < 1$, $K > 0$, and that*

$$Q(x) \notin \mathscr{C} \quad \text{for all } x \in \partial B^2_R.$$

If the homotopy class of $\mathscr{R}(Q_{|\partial B^2_R})$ is non-trivial, then

$$E_\varepsilon(Q, B^2_R) + C\,R\,E_\varepsilon(Q, \partial B^2_R) \geq \kappa_* \log \frac{R}{\varepsilon} - C,$$

for a constant $C = C(K)$.

Proof. We apply Proposition 2.2.5 to the map $\tilde{Q} \in H^1(B^2_{2R}, \mathbf{S}_0)$ defined by

$$\tilde{Q}(x) := \begin{cases} Q\left(\dfrac{Rx}{|x|}\right) & \text{if } x \in B^2_{2R} \setminus B^2_R \\ Q(x) & \text{if } x \in B^2_R, \end{cases}$$

and notice that

$$E_\varepsilon(\tilde{Q}, B^2_{2R}) \leq E_\varepsilon(Q, B^2_R) + C\,R\,E_\varepsilon(Q, \partial B^2_R). \qquad \square$$

Consider for a moment a complex-valued map u, defined on a domain $U \subseteq \mathbb{R}^k$. The gradient of u can be decomposed in terms of modulus and phase, that is,

$$|\nabla u|^2 = |\nabla |u||^2 + |u|^2 \left|\nabla \left(u/|u|\right)\right|^2 \qquad \text{a.e. on } U.$$

In a similar way, the energy of a map $\Omega \to \mathbf{S}_0$ is controlled from below by the energy of $\phi \circ Q$ (which plays the role of the modulus) and $\mathscr{R} \circ Q$ (in place of the phase).

Lemma 2.2.7. *Let $U \subseteq \mathbb{R}^k$ be a domain and let $Q \in C^1(U, \mathbf{S}_0)$. The function $\mathscr{R} \circ Q$ is well-defined and of class C^1 on the open set $Q^{-1}(\mathbf{S}_0 \setminus \mathscr{C}) \subseteq U$, and*

$$|\nabla Q|^2 \geq \frac{s_*^2}{3} \left|\nabla\left(\phi \circ Q\right)\right|^2 + \left(\phi \circ Q\right)^2 \left|\nabla\left(\mathscr{R} \circ Q\right)\right|^2 \qquad \text{on } U \tag{2.2.8}$$

(where we have set $(\phi \circ Q)|\nabla(\mathscr{R} \circ Q)|(x) := 0$ if $Q(x) \in \mathscr{C}$).

Proof. Because of our choice of the norm, we have

$$|\nabla \psi|^2 = \sum_{i=1}^k |\partial_{x_i} \psi|^2 \tag{2.2.9}$$

for any scalar or tensor-valued map ψ. Thus, it suffices to prove the inequality where ∇ is replaced by the partial derivative operator ∂_{x_i}, then sum over $i = 1, \ldots, k$. In view of this remark, without loss of generality we assume that $k = 1$.

Since ϕ is Lipschitz continuous, we know that $\phi \circ Q \in W^{1,\infty}_{\mathrm{loc}}(U)$ and $\phi \circ Q = 0$ on $Q^{-1}(\mathscr{C})$. Therefore, for a.e. $x \in Q^{-1}(\mathscr{C})$ we have $(\phi \circ Q)'(x) = 0$ and (2.2.8) is trivially satisfied at x. For the rest of the proof, we fix a point $x \in U \setminus Q^{-1}(\mathscr{C})$ so $\phi \circ Q$ is of class C^1 in a neighborhood of x.

Suppose that $r(Q(x)) > 0$. In this case, all the eigenvalues of $Q(x)$ have multiplicity 1. Using Lemma 2.2.1 and the results in [8], the map Q can be locally written as

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) + sr\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right), \tag{2.2.10}$$

where s, r, $\mathbf{n}$, $\mathbf{m}$ are C^1 functions defined in a neighborhood of x, satisfying the constraints

$$s > 0, \qquad 0 < r < 1, \qquad |\mathbf{n}| = |\mathbf{m}| = 1, \qquad \mathbf{n} \cdot \mathbf{m} = 0.$$

Then,

$$\mathscr{R} \circ Q = s_* \left(\mathbf{n}^{\otimes 2} - \frac{1}{3} \operatorname{Id} \right) \tag{2.2.11}$$

so $\mathscr{R} \circ Q$ is of class C^1 in a neighborhood of x, and we can use (2.2.10), (2.2.11) to compute $|Q'|$, $|(\mathscr{R} \circ Q)'|$. Setting $t := sr$, a straightforward computation gives

$$s_*^2 (\phi \circ Q)'^2 = s'^2 - 2s't' + t'^2, \qquad |(\mathscr{R} \circ Q)'|^2 = 2s_*^2 |\mathbf{n}'|^2 \tag{2.2.12}$$

and

$$\begin{aligned} |Q'|^2 &= \frac{2}{3} \left(s'^2 - s't' + t'^2 \right) + 2s^2 |\mathbf{n}'|^2 + 2t^2 |\mathbf{m}'|^2 + 4st(\mathbf{n}' \cdot \mathbf{m})(\mathbf{n} \cdot \mathbf{m}') \\ &\geq \frac{s_*^2}{3} (\phi \circ Q)'^2 + 2s^2 \left(|\mathbf{n}'|^2 + r^2 |\mathbf{m}'|^2 + 2r(\mathbf{n}' \cdot \mathbf{m})(\mathbf{n} \cdot \mathbf{m}') \right) \end{aligned} \tag{2.2.13}$$

Let $\mathbf{p} := \mathbf{n} \times \mathbf{m}$, so that $(\mathbf{n}, \mathbf{m}, \mathbf{p})$ is an orthonormal, positive frame in $\mathbb{R}^3$. By differentiating the orthogonality conditions for $(\mathbf{n}, \mathbf{m}, \mathbf{p})$, we obtain

$$\begin{cases} \mathbf{n}' = \alpha \mathbf{m} + \beta \mathbf{p} \\ \mathbf{m}' = -\alpha \mathbf{n} + \gamma \mathbf{p} \end{cases}$$

for some smooth, real-valued functions α, β, γ. Then, from (2.2.13) and (2.2.12) we deduce

$$\begin{aligned} |Q'|^2 - \frac{s_*^2}{3} (\phi \circ Q)'^2 &\geq 2s^2 \left(\alpha^2 + \beta^2 + r^2 (\alpha^2 + \gamma^2) - 2r\alpha^2 \right) \\ &\geq 2s^2 (1 - r)^2 (\alpha^2 + \beta^2) \\ &= \frac{s^2 (1 - r)^2}{s_*^2} |(\mathscr{R} \circ Q)'|^2 = (\phi \circ Q)^2 |(\mathscr{R} \circ Q)'|^2 , \end{aligned}$$

so (2.2.8) holds at the point x.

If $r(Q) = 0$ in a neighborhood of x then the function $\mathbf{m}$ in Formula (2.2.10) might not be well-defined. However, the previous computation still make sense because $t = sr$ vanishes in a neighborhood of x, and from (2.2.12), (2.2.13) we deduce that (2.2.8) holds at x.

We still have to consider a case, namely, $r(Q(x)) = 0$ but $r(Q)$ does not vanish identically in a neighborhood of x. In this case, there exists a sequence $x_k \to x$ such that $r(Q(x_k)) > 0$ for each $k \in \mathbb{N}$. By the previous discussion (2.2.8) holds at each x_k, and the functions $\phi \circ Q$, P' are continuous (by Lemmas 2.2.3 and 2.2.2). Passing to the limit as $k \to +\infty$, we conclude that (2.2.8) is satisfied at x as well. $\square$

Remark 2.2.2. Lemma 2.2.7 holds true, with the same proof, when U is a 1-dimensional manifold. When U is a Riemann manifold of dimension k, the equality (2.2.9) may not be true but $|\nabla \psi|^2$ is still controlled from below by the sum of $|\partial_{x_i} \psi|^2$. Therefore, we obtain an inequality similar to (2.2.8), where the right-hand side is multiplied by a constant factor $C \neq 1$. This constant depends on k and on the choice of metric.

The regularity of Q in Lemma 2.2.7 can be relaxed. We give an independent statement of this fact, since it will be useful later.

Corollary 2.2.8. *The map $\tau \colon \mathbf{S}_0 \to \mathbf{S}_0$ given by*

$$\tau \colon Q \mapsto \begin{cases} s_* \phi(Q) \mathscr{R}(Q) & \text{if } Q \in \mathbf{S}_0 \setminus \mathscr{C} \\ 0 & \text{if } Q \in \mathscr{C} \end{cases}$$

is Lipschitz-continuous. Moreover, for any $Q \in H^1(U, \mathbf{S}_0)$ there holds $\tau \circ Q \in H^1(U, \mathbf{S}_0)$ and

$$|\nabla Q|^2 \geq \frac{s_*^2}{3} |\nabla (\phi \circ Q)|^2 + (\phi \circ Q)^2 |\nabla (\mathscr{R} \circ Q)|^2 \geq \frac{1}{4} |\nabla (\tau \circ Q)|^2 \qquad \mathscr{H}^k\text{-a.e. on } U. \tag{2.2.14}$$

Proof. By differentiating τ, and by applying (2.2.8) to the map $Q = \mathrm{Id}_{\mathbf{S}_0}$, we obtain

$$\frac{1}{4}|\mathrm{D}\tau|^2 \leq \frac{s_*^2}{3}|\mathrm{D}\phi|^2 + \phi^2|\mathrm{D}\mathscr{R}|^2 \leq C \qquad \text{on } \mathbf{S}_0 \setminus \mathscr{C}.$$

Using this uniform bound, together with $\tau \in C(\mathbf{S}_0, \mathbf{S}_0)$ and $\tau_{|\mathscr{C}} = 0$, it is not hard to conclude that τ has bounded derivative in the sense of distributions, therefore τ is a Lipschitz function and the lower bound in (2.2.14) holds. The upper bound follows easily by a density argument. Let $\{Q^j\}_{j\in\mathbb{N}}$ be a sequence of smooth maps such that $Q^j \to Q$, $\nabla Q^j \to \nabla Q$. Using the regularity of $\mathscr{R}$ and ϕ on $\mathbf{S}_0 \setminus \mathscr{C}$ (Lemmas 2.2.2 and 2.2.3), we deduce $\nabla(\mathscr{R}\circ Q^j) \to \nabla(\mathscr{R}\circ Q)$ and $\nabla(\phi\circ Q^j) \to \nabla(\phi\circ Q)$ a.e. on $Q^{-1}(\mathbf{S}_0\setminus\mathscr{C})$, so (2.2.14) holds a.e. on $Q^{-1}(\mathbf{S}_0\setminus\mathscr{C})$. On the other hand, $\nabla(\phi\circ Q) = 0$ a.e. on $Q^{-1}(\mathscr{C}) = (\phi\circ Q)^{-1}(0)$, thus (2.2.14) holds trivially on $U \setminus Q^{-1}(\mathbf{S}_0\setminus\mathscr{C})$. □

In Chapter 1, Subsection 1.2.1, we have associated with each homotopy class $\gamma \in \Gamma(\mathscr{N})$ a number $\lambda_*(\gamma)$, which measures the energy cost of that class. This was useful in order to obtain Jerrard-Sandier type estimates (see Chapter 1, Subsection 1.4.2). In case the underlying manifold is the real projective plane, quantifying the energy cost of homotopically non-trivial maps is simple, because there is a unique class of such maps. Define

$$\kappa_* := \inf\left\{\frac{1}{2}\int_{\mathbb{S}^1}|P'(\theta)|^2\,\mathrm{d}\theta\colon P \in H^1(\mathbb{S}^1, \mathscr{N}) \text{ is non homotopically trivial}\right\}. \tag{2.2.15}$$

(Using the notation of Chapter 1, we have $\kappa_* = \lambda_*(\gamma)$ where γ is the non-trivial class.) Thanks to the compact embedding $H^1(\mathbb{S}^1, \mathscr{N}) \hookrightarrow C^0(\mathbb{S}^1, \mathscr{N})$, it is easy to check that the infimum is achieved. Moreover, minimizers are geodesic in $\mathscr{N}$. We have the following property, which has been proved in Chapter 1, Lemma 1.3.4.

Lemma 2.2.9. *We have*

$$\kappa_* = \frac{\pi}{2}s_*^2$$

and a minimizer for (2.2.15) *is given by*

$$P(\theta) := s_*\left(\mathbf{n}_*(\theta)^{\otimes 2} - \frac{1}{3}\mathrm{Id}\right) \qquad \text{for } 0 \leq \theta \leq 2\pi,$$

where $\mathbf{n}_*(\theta) := (\cos(\theta/2), \sin(\theta/2), 0)^{\mathsf{T}}$.

Combining the previous results, we obtain a lower bound for the energy on circles (compare to [75, Theorem 2.1, Corollary 2.1]).

Lemma 2.2.10. *For $\rho > 1$, let $Q \in C^1(\partial B^2_\rho, \mathbf{S}_0)$ satisfy*

$$Q(x) \notin \mathscr{C} \qquad \text{for all } x \in \partial B^2_\rho.$$

If the homotopy class of $\mathscr{R}(Q_{|\partial B^2_\rho})$ is non-trivial, then

$$E_1(Q, \partial B^2_\rho) \geq \kappa_*\rho^{-1} - C\rho^{-3/2},$$

where the constant C depends only on f, $\|Q\|_{L^\infty(\partial B^2_\rho)}$ and $\|\nabla Q\|_{L^\infty(\partial B^2_\rho)}$.

Proof. Set

$$K := \max\left\{\|Q\|_{L^\infty(\partial B^2_\rho)}, \|\nabla Q\|_{L^\infty(\partial B^2_\rho)}\right\}, \qquad m := \min_{\partial B^2_\rho}\phi(Q) > 0,$$

and let $x_0 \in \partial B^2_\rho$ be a point where the minimum of $\phi(Q)$ is attained. Suppose, at first, that $m < 1$. Then, it is clear that

$$\phi(Q) \leq \frac{1+m}{2} \qquad \text{on } B^2_{\rho_0}(x_0), \tag{2.2.16}$$

where

$$\rho_0 := \frac{1-m}{2\left\|\nabla\phi(Q)\right\|_{L^\infty}}.$$

Since ϕ is locally Lipschitz continuous, by Lemma 2.2.3, we have

$$\rho_0 \geq C\frac{1-m}{\left\|\nabla Q\right\|_{L^\infty}} \geq CK^{-1}(1-m),$$

which yields

$$\mathscr{H}^1(\partial B^2_\rho \cap B^2_{\rho_0}(x_0)) \geq C\rho_0 \geq CK^{-1}(1-m) \tag{2.2.17}$$

because $\rho \geq 1$. Thus, using (2.2.16), (2.2.17) and (F_1), we have

$$\int_{\partial B^2_\rho} f(Q)\,\mathrm{d}\mathscr{H}^1 \geq C_K\left(1-\frac{1+m}{2}\right)^2 \mathscr{H}^1(\partial B^2_\rho \cap B^2_{\rho_0}(x_0)) \geq C_K(1-m)^3. \tag{2.2.18}$$

We denote by C_K a positive constant which depends depending only on f, K.

On the other hand, $P := \mathscr{R}(Q_{|\partial B^2_\rho})$ is well-defined, and is a non-homotopically trivial loop in $\mathscr{N}$. Suppose for a moment that $\rho = 1$. Then, using Lemma 2.2.7 and (2.2.15), we have

$$\frac{1}{2}\int_{\mathbb{S}_1} |\nabla Q|^2\,\mathrm{d}\mathscr{H}^1 \geq \frac{1}{2}\int_{\partial B^2_1} |\nabla_\top Q|^2\,\mathrm{d}\mathscr{H}^1 \geq \frac{m^2}{2}\int_{\partial B^2_1} |\nabla_\top P|^2\,\mathrm{d}\mathscr{H}^1 \geq \kappa_* m^2,$$

where we denote by $\nabla_\top$ the tangential derivation. For a general $\rho \geq 1$, by a scaling argument we obtain

$$\frac{1}{2}\int_{\partial B^2_\rho} |\nabla Q|^2\,\mathrm{d}\mathscr{H}^1 \geq \frac{\kappa_* m^2}{\rho}. \tag{2.2.19}$$

Combining (2.2.18) and (2.2.19), we have

$$E_1(Q,\, \partial B^2_\rho) \geq \min_{0\leq m\leq 1}\left\{\frac{\kappa_* m^2}{\rho} + C_K(1-m)^3\right\}. \tag{2.2.20}$$

By elementary calculus, we see that the function $m \mapsto \kappa_* m^2\rho^{-1} + C_K(1-m)^3$ has a unique minimum m_0 in the interval $[0,\,1]$, and that

$$\frac{2\kappa_* m_0}{\rho} = 3C_K(1-m_0)^2.$$

This implies

$$\frac{3C_K\rho}{2\kappa_*}(1-m_0)^2 = m_0 \leq 1,$$

whence

$$m_0 \geq 1 - \sqrt{\frac{2\kappa_*}{3C_K\rho}}$$

and

$$\min_{0\leq m\leq 1}\left\{\frac{\kappa_* m^2}{\rho} + C_K(1-m)^3\right\} \geq \frac{\kappa_*}{\rho}\left(1-\sqrt{\frac{2\kappa_*}{3C_K\rho}}\right)^2 \geq \kappa_*\rho^{-1} - C_K\rho^{-3/2}.$$

Injecting this inequality in (2.2.20), we conclude the proof, in case $m < 1$. On the other hand, when $m \geq 1$ the proof of (2.2.19) remains valid, and in this case (2.2.19) immediately implies the lemma. $\square$

Finally, we can prove the main result of this subsection.

Proof of Proposition 2.2.5. We can assume without loss of generality that Q is of class C^1, by a density argument. Moreover, we are going to scale the variables, so that we reduce to the case $\varepsilon = 1$. Define $u_\varepsilon \colon B_{R/\varepsilon} \to \mathbf{S}_0$ by

$$u_\varepsilon(x) := Q(\varepsilon x) \qquad \text{for } x \in B_{R/\varepsilon}. \tag{2.2.21}$$

By the assumptions on Q,

$$\|u_\varepsilon\|_{L^\infty(B_{R/\varepsilon})} + \|\nabla u_\varepsilon\|_{L^\infty(B_{R/\varepsilon})} \leq K, \qquad E_1(u_\varepsilon,\, B^2_{R/\varepsilon}) = E_\varepsilon(Q_\varepsilon,\, B^2_R).$$

There exists a constant $C_* = C_*(K)$ such that

$$E_1(u_\varepsilon,\, B^2_1(x)) \geq 4C_* \qquad \text{as soon as } u_\varepsilon(x) \in \mathscr{C}. \tag{2.2.22}$$

Indeed, if $u_\varepsilon(x) = 0$ then $\phi(u_\varepsilon) \leq 1/2$ on a ball of radius $(2\|\nabla\phi(u_\varepsilon)\|)^{-1} \geq CK^{-1}$, so (2.2.22) follows by (F_1). We also set

$$\Lambda(r) := \int_0^r \min\left\{C_*,\, \kappa_*\rho^{-1} - C\rho^{-3/2}\right\} \mathrm{d}s \qquad \text{for } r > 0,$$

where C is exactly the constant which appear in Lemma 2.2.10. Now assume, for instance, that $\mathscr{R}(u_\varepsilon)_{|\partial B_r}$ is well-defined and not trivial for a.e. $r \in [R_1,\, R_2]$, and $1 \leq R_1 < R_2 \leq R/\varepsilon$. Then, by integrating Lemma 2.2.10, we obtain

$$E_1(u_\varepsilon,\, B^2_{R_2} \setminus B^2_{R_1}) \geq \Lambda(R_2) - \Lambda(R_1) \geq \kappa_* \log(R_2/R_1) - C(K).$$

The proposition follows a covering argument, as in [75, Theorems 3.1 and 4.1]. We do not detail it here, as the proof of [75] applies word by word. ◻

2.2.3 Basic properties of minimizers

We conclude the preliminary section by recalling recall some basic facts about minimizers of (LG_ε).

Lemma 2.2.11. *Minimizers Q_ε of* (LG_ε) *exist and are of class C^∞ in the interior of Ω. Moreover, for any $U \subset\subset \Omega$ they satisfy*

$$\|Q_\varepsilon\|_{L^\infty(U)} + \varepsilon\,\|\nabla Q_\varepsilon\|_{L^\infty(U)} \leq C(U).$$

Sketch of the proof. The existence of minimizers follows by standard method in Calculus of Variations. Minimizers solve the Euler-Lagrange system

$$-\varepsilon^2 \Delta Q_\varepsilon - aQ_\varepsilon - bQ_\varepsilon^2 + \frac{b}{3}\,\mathrm{Id}\,|Q_\varepsilon|^2 + c\,|Q_\varepsilon|^2\, Q_\varepsilon = 0 \tag{2.2.23}$$

on Ω, in the sense of distributions. The term $\mathrm{Id}\,|Q_\varepsilon^2|$ is a Lagrange multiplier, associated with the tracelessness constraint. The elliptic regularity theory, combined with the uniform L^∞-bound of Assumption (H), implies that each component $Q_{\varepsilon,ij}$ is of class C^∞ in the interior of the domain. The $W^{1,\infty}(U)$-bound follows by interpolation results, see [13, Lemma A.1, A.2]. ◻

Lemma 2.2.12 (Monotonicity formula)**.** *Let $x_0 \in \Omega$, and let $0 < r_1 < r_2 < \mathrm{dist}(x_0,\, \partial\Omega)$. Then*

$$r_1^{-1} E_\varepsilon(Q_\varepsilon,\, B_{r_1}(x_0)) \leq r_2^{-1} E_\varepsilon(Q_\varepsilon,\, B_{r_2}(x_0)).$$

Proof. This formula is proved in [98, Lemma 2], but we give here the proof for the sake of completeness. The monotonicity formula follows from the Pohozaev identity, which has been proved in Chapter 1. Taking $n = 3$ and $G = B_r(x_0) \subseteq \mathbb{R}^3$ in Lemma 1.4.2, the Pohozaev identity writes

$$E_\varepsilon(Q_\varepsilon,\, B_r(x_0)) + \frac{r}{2}\int_{\partial B_r(x_0)} \left|\frac{\partial Q_\varepsilon}{\partial\nu}\right|^2 \mathrm{d}\mathscr{H}^1 = r\, E_\varepsilon(Q_\varepsilon,\, \partial B_r(x_0)). \tag{2.2.24}$$

In particular, we have

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{E_\varepsilon(Q_\varepsilon,\, B_r(x_0))}{r}\right) = \frac{1}{r^2}\Big(r\, E_\varepsilon(Q_\varepsilon,\, \partial B_r(x_0)) - E_\varepsilon(Q_\varepsilon,\, B_r(x_0))\Big)$$
$$\overset{(2.2.24)}{=} \frac{1}{2r}\int_{\partial B_r(x_0)} \left|\frac{\partial Q_\varepsilon}{\partial \nu}\right|^2 \mathrm{d}\mathscr{H}^1 \geq 0,$$

whence the lemma follows. □

Lemma 2.2.13 (Stress-energy identity)**.** *For any $i \in \{1,\ 2,\ 3\}$, the minimizers satisfy*

$$\frac{\partial}{\partial x_j}\left(e_\varepsilon(Q_\varepsilon)\delta_{ij} - \frac{\partial Q_\varepsilon}{\partial x_i}\cdot\frac{\partial Q_\varepsilon}{\partial x_j}\right) = 0 \qquad \text{in } \Omega$$

in the sense of distributions.

Proof. Since Q_ε is of class C^∞ in the interior of the domain by Lemma 2.2.11, we can differentiate the products and use the chain rule. Setting $\partial_i := \partial/\partial x_i$ for the sake of brevity, for each i we have

$$\begin{aligned}
&\partial_j\big(e_\varepsilon(Q_\varepsilon)\delta_{ij} - \partial_i Q_\varepsilon \cdot \partial_j Q_\varepsilon\big) \\
&\qquad = \partial_i\partial_k Q_\varepsilon \cdot \partial_k Q_\varepsilon + \frac{1}{\varepsilon^2}\frac{\partial f(Q_\varepsilon)}{\partial Q_{pq}}\partial_i Q_{\varepsilon,pq} - \partial_i\partial_j Q_\varepsilon \cdot \partial_j Q_\varepsilon - \partial_i Q_\varepsilon \cdot \partial_j\partial_j Q_\varepsilon \\
&\qquad \overset{(2.2.23)}{=} \partial_k\partial_k Q_\varepsilon \cdot \partial_i Q_\varepsilon - \frac{b}{3}\left|Q_\varepsilon\right|^2 \mathrm{Id}\cdot\partial_i Q_\varepsilon - \partial_i Q_\varepsilon \cdot \partial_j\partial_j Q_\varepsilon = 0
\end{aligned}$$

where we have used that $\mathrm{Id}\cdot\partial_i Q_\varepsilon = 0$, because Q_ε is traceless. □

2.3 Extension properties

2.3.1 Extension of $\mathbb{S}^2$-valued maps

In some of our arguments, we will encounter extension problems for $\mathscr{N}$-valued maps. This means, given $g\colon \partial B^k_r \to \mathscr{N}$ (for $k \in \mathbb{N}$, $k \geq 2$ and $r > 0$) we look for a map $Q\colon B^k_r \to \mathscr{N}$ satisfying $Q_{|\partial B^k_r} = g$, with a control on the energy of Q. When the datum g is regular enough (say, of class C^1) and satisfies some topological condition, this problem can be reformulated in terms of $\mathbb{S}^2$-valued maps. Indeed, if the homotopy class of g is trivial then g can be *lifted*, i.e. there exists a map $\mathbf{n}\colon \partial B^k_r \to \mathbb{S}^2$, as regular as g, such that the diagram

$$\begin{tikzcd}
 & \mathbb{S}^2 \arrow[d, "\psi"] \\
\partial B^k_r \arrow[ur, "\mathbf{n}"] \arrow[r, "g"'] & \mathscr{N}
\end{tikzcd}$$

commutes. Here ψ is the universal covering map of $\mathscr{N}$, given by

$$\psi(\mathbf{n}) := s_*\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) \qquad \text{for } \mathbf{n} \in \mathbb{S}^2.$$

In other words, the function $\mathbf{n}$ satisfies to

$$g(x) = (\psi \circ \mathbf{n})(x) \qquad \text{for (almost) every } x \in \partial B^k_r. \tag{2.3.1}$$

As $\mathbb{S}^2$ is a simply connected manifold, $\mathbb{S}^2$-valued maps are easier to deal with than $\mathscr{N}$-valued map.

Hardt, Kinderlehrer and Lin proposed, in their paper [60], an interesting argument for constructing extensions of $\mathbb{S}^2$-valued maps. They combined $\mathbb{R}^3$-valued harmonic extensions with an average argument, in order to find a suitable re-projection $\mathbb{R}^3 \to \mathbb{S}^2$. For the convenience of the reader, in this subsection we recall briefly their proof. As a corollary, we recover extension results for $\mathscr{N}$-valued maps, which will be crucial in the proof of Proposition 2.1.6. In Section 2.5, a similar argument will be applied to an extension problem for $\mathbf{S}_0$-valued maps. This will be useful in the proof of Proposition 2.1.3.

Lemma 2.3.1. *For any $r > 0$, $k \geq 3$ and any $g \in H^1(\partial B^k_r, \mathscr{N})$, there exists $P \in H^1(B^k_r, \mathscr{N})$ which satisfies $P_{|\partial B^k_r} = g$ and*

$$\int_{B^k_r} |\nabla P|^2 \, \mathrm{d}\mathscr{H}^2 \leq C r^{k/2-1/2} \left(\int_{\partial B^k_r} |\nabla_\top g|^2 \, \mathrm{d}\mathscr{H}^1 \right)^{1/2}$$

for a constant C is independent of g, r.

Lemma 2.3.2. *There exists a constant $C > 0$ such that, for any $r > 0$ and any $g \in H^1(B^2_r, \mathscr{N})$, there exists $P \in H^1(B^2_h, \mathscr{N})$ satisfying $P_{|\partial B^2_r} = g$ and*

$$\int_{B^2_r} |\nabla P|^2 \, \mathrm{d}\mathscr{H}^2 \leq C r \int_{\partial B^2_r} |\nabla_\top g|^2 \, \mathrm{d}\mathscr{H}^1,$$

where C is independent of g, r.

In Lemma 2.3.1, the two sides of the inequality have different homogeneities in v, g. This fact is of main importance, for the arguments of Section 2.4 rely crucially on it. For the case $k = 2$ (Lemma 2.3.1), we need to assume that g is defined over the whole of B^2_r, because ∂B^2_r is not simply connected.

Throughout the subsection, we assume that $\mathbf{n} \in H^1(\partial B^k_r, \mathbb{S}^2)$, for some $r > 0$ and $k \geq 2$. We let $\mathbf{w}$ be the ($\mathbb{R}^3$-valued) harmonic extension of $\mathbf{n}$, i.e. the unique solution $\mathbf{w} \in H^1(B^k_r, \mathbb{R}^3)$ to

$$\begin{cases} -\Delta \mathbf{w} = 0 & \text{on } B^k_r \\ \mathbf{w} = \mathbf{n} & \text{on } \partial B^k_r. \end{cases} \tag{2.3.2}$$

For the reader's convenience, we recall some classical facts.

Lemma 2.3.3. *The harmonic extension satisfies*

$$\int_{B^k_r} |\nabla \mathbf{w}|^2 \, \mathrm{d}\mathscr{H}^k \leq C_k r \int_{\partial B^k_r} |\nabla_\top \mathbf{n}|^2 \, \mathrm{d}\mathscr{H}^{k-1} \tag{2.3.3}$$

and

$$\int_{B^k_r} |\nabla \mathbf{w}|^2 \, \mathrm{d}\mathscr{H}^k \leq C_k \left(\int_{\partial B^k_r} |\nabla_\top \mathbf{n}|^2 \, \mathrm{d}\mathscr{H}^{k-1} \right)^{1/2}, \tag{2.3.4}$$

for a constant C_k depending only on k.

Sketch of the proof. Both the assertions follows by Pohozaev's identity

$$r \int_{\partial B^k_r} |\nabla_\top \mathbf{w}|^2 \, \mathrm{d}\mathscr{H}^{k-1} = \int_{B^k_r} |\nabla \mathbf{w}|^2 \, \mathrm{d}\mathscr{H}^k + r \int_{\partial B^k_r} \left| \frac{\partial \mathbf{w}}{\partial r} \right|^2 \mathrm{d}\mathscr{H}^{k-1}. \tag{2.3.5}$$

This identity can be derived formally by multiplying both sides of (2.3.2) with $x \cdot \nabla \mathbf{w}$ and integrating by parts on B^k_r. Inequality (2.3.3) (with $C_k = 1$) follows immediately from (2.3.5). For (2.3.4), we integrate by parts and use the Hölder inequality:

$$\int_{B^k_r} |\nabla \mathbf{w}|^2 \, \mathrm{d}\mathscr{H}^k \overset{(2.3.2)}{=} \int_{\partial B^k_r} \mathbf{w} \frac{\partial \mathbf{w}}{\partial r} \, \mathrm{d}\mathscr{H}^{k-1} \leq C_k \left(\int_{\partial B^k_r} \left| \frac{\partial \mathbf{w}}{\partial r} \right|^2 \mathrm{d}\mathscr{H}^{k-1} \right)^{1/2}.$$

But (2.3.5) implies that

$$\int_{\partial B_r^k} \left|\frac{\partial \mathbf{w}}{\partial r}\right|^2 \mathrm{d}\mathscr{H}^{k-1} \leq \int_{\partial B_r^k} |\nabla_\top \mathbf{w}|^2 \,\mathrm{d}\mathscr{H}^{k-1},$$

hence (2.3.4) follows. ☐

Lemma 2.3.4 (Hardt, Kinderlehrer and Lin, [60])**.** *For all* $\mathbf{n} \in H^1(\partial B_r^k, \mathbb{S}^2)$*, there exists an extension* $\tilde{\mathbf{w}} \in H^1(B_r^k, \mathbb{S}^2)$ *which satisfy* $\tilde{\mathbf{w}}_{|\partial B_r^k} = \mathbf{n}$*, (2.3.3) and (2.3.4).*

Proof. Let $\mathbf{w}$ be the harmonic extension of $\mathbf{n}$. Then $\mathbf{w}$ satisfies (2.3.3) and (2.3.4), but its image may not lie in $\mathbb{S}^2$. Thus, we consider the projection

$$\pi_a(x) := \frac{x-a}{|x-a|}, \qquad \text{for } x \in \mathbb{R}^3,$$

where $a \in B_{1/2} \subseteq \mathbb{R}^3$ is a fixed parameter. By elliptic regularity, $\mathbf{w}$ is of class C^∞ in the interior of B_r^k. Then Sard's lemma applies, and $\mathbf{w}^{-1}(a)$ is a $(k-3)$-submanifold of B_2^k for a.e. $a \in B_{1/2}$ (or $\mathbf{w}^{-1}(a)$ is empty for a.e. $a \in B_{1/2}$, when $k = 2$). Moreover, $\pi_a \circ \mathbf{w} \in C^\infty(B_r^k \setminus \mathbf{w}^{-1}(a), \mathbb{S}^2)$ so it makes sense to write

$$\begin{aligned}\int_{B_{1/2}} \int_{B_r^k} |\nabla(\pi_a \circ \mathbf{w})(x)|^2 \,\mathrm{d}\mathscr{H}^k(x)\,\mathrm{d}a &\leq 2\int_{B_r^k} |\nabla \mathbf{w}(x)|^2 \int_{B_{1/2}} |\mathbf{w}(x) - a|^{-2} \,\mathrm{d}a\,\mathrm{d}\mathscr{H}^k(x) \\ &= 8\pi \int_{B_r^k} |\nabla \mathbf{w}(x)|^2 \,\mathrm{d}\mathscr{H}^k(x).\end{aligned}$$

The integral has been estimated with Fubini-Tonelli's theorem and the change of variable $y = \mathbf{w}(x) - a$. By Fubini-Lebesgue theorem, we conclude that $\pi_a \circ \mathbf{w} \in H^1(B_r^k, \mathbb{S}^2)$ for a.e. $a \in B_{1/2}$, and by an average argument we find $a \in B_{1/2}$ such that

$$\int_{B_1^2} |\nabla(\pi_a \circ \mathbf{w})(x)|^2 \,\mathrm{d}\mathscr{H}^k(x) \leq C \int_{B_1^2} |\nabla \mathbf{w}(x)|^2 \,\mathrm{d}\mathscr{H}^k(x).$$

Then, the map

$$\tilde{\mathbf{w}} := \left(\pi_{a|\mathbb{S}^2}\right)^{-1} \circ \pi_a \circ \mathbf{w}$$

satisfies the lemma. ☐

We state now a lifting property for Sobolev maps. This subject has been studied extensively, among others, by Bethuel and Zheng [19], Bourgain, Brezis and Mironescu [20], Bethuel and Chiron [16], Ball and Zarnescu [10] (in particular, in the latter a problem closely related to the Q-tensor theory is considered).

Lemma 2.3.5. *Let* $\mathscr{M}$ *be a smooth, simply connected surface (possibly with boundary). Then, any map* $g \in H^1(\mathscr{M}, \mathscr{N})$ *has a lifting, i.e. there exists* $\mathbf{n} \in H^1(\mathscr{M}, \mathbb{S}^2)$ *which satisfies* (2.3.1)*. Moreover,*

$$|\nabla g|^2 = 2s_*^2 |\nabla \mathbf{n}|^2 \qquad \mathscr{H}^2\text{-a.e. on } \mathscr{M}. \tag{2.3.6}$$

If $\mathscr{M}$ *has a boundary then* $\mathbf{n}_{|\partial\mathscr{M}}$ *is a lifting of* $g_{|\partial\mathscr{M}}$*, and if* $g_{|\partial\mathscr{M}} \in H^1(\partial\mathscr{M}, \mathscr{N})$ *then* $\mathbf{n}_{|\partial\mathscr{M}} \in H^1(\partial\mathscr{M}, \mathbb{S}^2)$*.*

Proof. The identity (2.3.6) follows directly by (2.3.1), by a straightforward computation. The existence of a lifting is a well-known topological fact, when g is of class C^1. In case $g \in H^1$ and $\mathscr{M}$ is a bounded, smooth domain in $\mathbb{R}^n$, the existence of a lifting has been proved by Ball and Zarnescu [10]. Another possibility is to argue by density of smooth maps in $H^1(\mathscr{M}, \mathscr{N})$ (see [126]). If $\mathscr{M}$ is a surface with boundary, one can use a density argument again to construct a lifting with the desidered properties. Actually, every H^1-lifting satisfies to the same regularity properties at the boundary. Indeed, if $\mathbf{n}_1$, $\mathbf{n}_2$ are two H^1-lifting of the same map, then $\mathbf{n}_1 \cdot \mathbf{n}_2$ is an H^1-map $\mathscr{M} \to \{1, -1\}$ and so, by a slicing argument, either $\mathbf{n}_1 = \mathbf{n}_2$ a.e. or $\mathbf{n}_1 = -\mathbf{n}_2$ a.e (see [10, Proposition 2]). ☐

Combining Lemmas 2.3.4 and 2.3.5, we obtain easily the results we need.

Proof of Lemmas 2.3.1 and 2.3.2. Consider Lemma 2.3.1 first. Let $\mathbf{n} \in H^1(\partial B_r^k, \mathbb{S}^2)$ be a lifting of g, whose existence is guaranteed by Lemma 2.3.5, and let $\tilde{\mathbf{w}} \in H^1(B_r^k, \mathbb{S}^2)$ be the extension given by Lemma 2.3.4. Then, the map defined by

$$P(x) := s_* \left(\tilde{\mathbf{w}}^{\otimes 2}(x) - \frac{1}{3} \operatorname{Id} \right) \qquad \text{for } \mathscr{H}^k\text{-a.e. } x \in B_r^k$$

has the desired properties. The proof of Lemma 2.3.2 is analogous. □

2.3.2 Luckhaus' lemma and its variants

When dealing with the asymptotic analysis for minimizers Q_ε of (LG$_\varepsilon$), we will be confronted with the following problem. We assume that $B_1 \subseteq \Omega$, and we aim to compare $E_\varepsilon(Q_\varepsilon, B_1)$ with the energy of a map $P_\varepsilon \colon B_1 \to \mathbf{S}_0$. However, it may be that $P_{\varepsilon|\partial B_1} \neq Q_{\varepsilon|\partial B_1}$, so P_ε is not an admissible comparison map. To correct this, we need to construct a function which interpolates between $P_{\varepsilon|\partial B_1}$ and $Q_{\varepsilon|\partial B_1}$ over a spherical shell.

In general terms, the problem may be stated as follows. Fix a parameter $0 < \epsilon < 1$, and consider two H^1-maps $u_\epsilon, v_\epsilon \colon \partial B_1 \to \mathbf{S}_0$. We aim at finding a spherical shell $A_\epsilon := B_1 \setminus B_{1-h(\epsilon)}$ of (small) thickness $h(\epsilon) > 0$ and a function $\varphi_\epsilon \colon A_\epsilon \to \mathbf{S}_0$, such that

$$\varphi_\epsilon(x) = u_\epsilon(x) \quad \text{and} \quad \varphi_\epsilon(x - h(\epsilon)x) = v_\epsilon(x) \qquad \text{for } \mathscr{H}^2\text{-a.e. } x \in \partial B_1 \tag{2.3.7}$$

and the energy $E_\varepsilon(\varphi_\epsilon, A_\epsilon)$ is controlled in terms of u_ϵ, v_ϵ. Additional assumptions on u_ϵ, v_ϵ are needed, otherwise the energy of φ_ϵ may become too large. Moreover, in some circumstances only the function u_ϵ is prescribed, and we will need to find *both* a map $v_\epsilon \colon \partial B_1 \to \mathscr{N}$ which approximates u_ϵ (in some sense to be made precise) and the interpolating function φ_ϵ.

Luckhaus proved an interesting interpolation lemma (see [92, Lemma 1]), which turned out to be useful for several applications. When the two maps u_ϵ, v_ϵ take values in the manifold $\mathscr{N}$, he constructed an extension φ_ϵ satisfying (2.3.7), with bounds on $\operatorname{dist}(\varphi_\epsilon, \mathscr{N})$ and on the Dirichlet integral

$$\int_{B_1 \setminus B_{1-h(\epsilon)}} |\nabla \varphi_\epsilon|^2 .$$

For the convenience of the reader, and for future reference, we recall Luckhaus' lemma. Since the potential $\epsilon^{-2} f$ is not taken into account here, we drop the subscript ϵ in the notation.

Lemma 2.3.6 (Luckhaus, [92])**.** *For any $\beta \in (1/2, 1)$, there exists a constant $c > 0$ with this property. For any fixed numbers $0 < \lambda \leq 1/2$, $0 < \sigma < 1$ and any $u, v \in H^1(\partial B_1, \mathscr{N})$, set*

$$K := \int_{\partial B_1} \left\{ |\nabla u|^2 + |\nabla v|^2 + \frac{|u - v|^2}{\sigma^2} \right\} \mathrm{d}\mathscr{H}^2.$$

Then, there exists a function $\varphi \in H^1(B_1 \setminus B_{1-\lambda}, \mathbf{S}_0)$ satisfying (2.3.7)*,*

$$\operatorname{dist}(\varphi(x), \mathscr{N}) \leq c\sigma^{1-\beta}\lambda^{-1/2}K^{1/2}$$

for a.e. $x \in B_1 \setminus B_{1-\lambda}$ and

$$\int_{B_1 \setminus B_{1-\lambda}} |\nabla \varphi|^2 \leq c\lambda \left(1 + \sigma^2\lambda^{-2}\right) K.$$

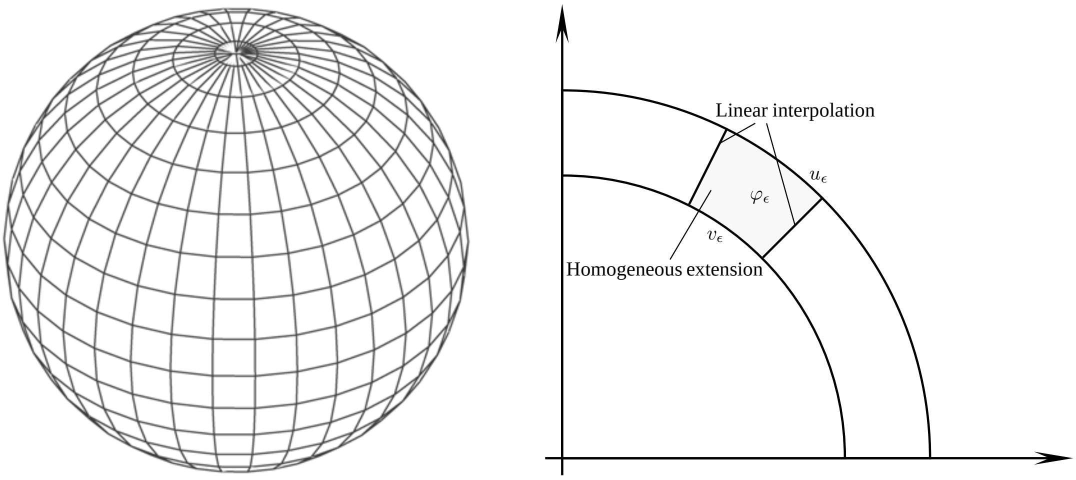


Figure 2.2: Left: a grid on a sphere. Right: the Luckhaus' construction. Given two maps u_ϵ, v_ϵ (respectively defined on the outer and inner boundary of a thin spherical shell), we construct a map φ_ϵ by using linear interpolation on the boundary of the cells, and homogeneous extension inside each cell.

The idea of the proof is illustrated in Figure 2.2. One constructs a grid on the sphere ∂B_1 with suitable properties. The map φ_ε is defined by linear interpolating between u_ε and v_ε on the boundary of the cells. Inside each cell, φ_ε is defined by a homogeneous extension. By choosing carefully the grid on ∂B_1, and using the Sobolev-Morrey embedding on the boundary of the cells, one can bound the distance between u_ε and v_ε on the 1-skeleton of the grid, in terms of κ. Then, the bound on the energy of φ_ε follows by a simple computation.

We will discuss here a couple of variants of this lemma. The first result deals with the case where only $u_\epsilon \colon \partial B_1 \to \mathbf{S}_0$ is prescribed. One needs then to find both $v_\epsilon \colon \partial B_1 \to \mathscr{N}$ and φ_ϵ. Approximating u_ϵ with a $\mathscr{N}$-valued function v_ϵ may be impossible, due to topological obstructions. However, this is possible if the energy of u_ϵ is small, compared to $|\log \epsilon|$. More precisely, we assume that

$$E_\epsilon(u_\epsilon, \partial B_1) \leq \eta_0 \, |\log \epsilon| \tag{2.3.8}$$

for some small constant $\eta_0 > 0$. For technical reasons, we also require a $W^{1,\infty}$-bound on u_ϵ, namely

$$\|u_\epsilon\|_{L^\infty(\partial B_1)} + \epsilon \, \|\mathrm{D} u_\epsilon\|_{L^\infty(\partial B_1)} \leq \kappa. \tag{2.3.9}$$

In our case of interest, where u_ϵ coincides with a minimizer of (LG$_\varepsilon$) restricted on a sphere, (2.3.9) is guaranteed by interior regularity estimates, see Lemma 2.2.11.

Proposition 2.3.7. *For any $\kappa > 0$, there exist positive numbers η_0, ϵ_1, C with the following property. For any $0 < \eta \leq \eta_0$, any $0 < \epsilon \leq \epsilon_1$ and any $u_\epsilon \in W^{1,\infty}(\partial B_1, \mathbf{S}_0)$ satisfying* (2.3.8)–(2.3.9)*, there exist maps $v_\epsilon \in H^1(\partial B_1, \mathscr{N})$, $\varphi_\epsilon \in H^1(B_1 \setminus B_{1-h(\epsilon)}, \mathbf{S}_0)$ which satisfy* (2.3.7)*,*

$$\frac{1}{2} \int_{\partial B_1} |\nabla v_\epsilon|^2 \, \mathrm{d}\mathscr{H}^2 \leq C E_\epsilon(u_\epsilon, \partial B_1), \tag{2.3.10}$$

$$E_\epsilon(\varphi_\epsilon, B_1 \setminus B_{1-h(\epsilon)}) \leq C h(\epsilon) E_\epsilon(u_\epsilon, \partial B_1) \tag{2.3.11}$$

for $h(\epsilon) := \epsilon^{1/2} |\log \epsilon|$.

We will discuss the proof of this proposition later on. Before that, we remark that v_ϵ is indeed an approximation of u_ϵ, i.e. their distance — measured in a suitable norm — tends to 0 as $\epsilon \to 0$.

Corollary 2.3.8. *Under the same assumptions of Proposition 2.3.7,*

$$\|u_\epsilon - v_\epsilon\|_{L^2(\partial B_1)} \leq C h^{1/2}(\epsilon) E_\epsilon^{1/2}(u_\epsilon, \partial B_1).$$

Proof. We can estimate the L^2-distance between u_n and v_n thanks to (2.3.7):

$$\begin{aligned}\|u_\epsilon - v_\epsilon\|^2_{L^2(\partial B_1)} &\overset{(2.3.7)}{=} \int_{\partial B_1} |\varphi_\epsilon(x) - \varphi_\epsilon(x - h(\epsilon)x)|^2 \, \mathrm{d}\mathscr{H}^2(x) \\ &= \int_{\partial B_1} \left| \int_{1-h(\epsilon)}^1 \nabla\varphi_\epsilon(tx)x \, \mathrm{d}t \right|^2 \mathrm{d}\mathscr{H}^2(x).\end{aligned}$$

Then, by Hölder inequality,

$$\begin{aligned}\|u_\epsilon - v_\epsilon\|^2_{L^2(\partial B_1)} &\leq h(\epsilon) \int_{\partial B_1} \int_{1-h(\epsilon)}^1 |\nabla\varphi_\epsilon(tx)|^2 \, \mathrm{d}t \, \mathrm{d}\mathscr{H}^2(x) \\ &\leq \frac{h(\epsilon)}{(1-h(\epsilon))^2} E_\epsilon(\varphi_\epsilon, \, B_1 \setminus B_{1-h(\epsilon)}) \overset{(2.3.11)}{\leq} Ch(\epsilon) E_\epsilon(u_\epsilon, \, \partial B_1).\end{aligned}$$ □

Combining Lemma 2.3.6 and Proposition 2.3.7, we obtain a third extension result. In this case, both the boundary values u, v are prescribed and, unlike Luckhaus' lemma, we provide a control over the potential energy of the extension $\epsilon^{-2} f(\varphi_\epsilon)$.

Proposition 2.3.9. *Let $\{\sigma_\epsilon\}_{\epsilon>0}$ be a positive sequence such that $\sigma_\epsilon \to 0$, and let u_ϵ, v_ϵ be given functions in $H^1(\partial B_1, \mathbf{S}_0)$. For all $\epsilon > 0$, assume that u_ϵ satisfies* (2.3.9)*, that $v_\epsilon(x) \in \mathscr{N}$ for $\mathscr{H}^2$-a.e. $x \in \partial B_1$ and that*

$$\int_{\partial B_1} \left\{ |\nabla u_\epsilon|^2 + \frac{1}{\epsilon^2} f(u_\epsilon) + |\nabla v_\epsilon|^2 + \frac{|u_\epsilon - v_\epsilon|^2}{\sigma_\epsilon^2} \right\} \mathrm{d}\mathscr{H}^2 \leq C \tag{2.3.12}$$

for an ϵ-independent constant C. Set

$$\nu_\epsilon := h(\epsilon) + \left(h^{1/2}(\epsilon) + \sigma_\epsilon \right)^{1/4} (1 - h(\epsilon)) \, .$$

Then, there exist a number $\epsilon_1 > 0$ and, for $0 < \epsilon \leq \epsilon_1$, a function $\varphi_\epsilon \in H^1(B_1 \setminus B_{1-\nu_\epsilon}, \mathbf{S}_0)$ which satisfies (2.3.7) *and*

$$E(\varphi_\epsilon, \, B_1 \setminus B_{1-\nu_\epsilon}) \leq C\nu_\epsilon.$$

The assumption (2.3.12) could be relaxed by requiring just a logarithmic bound, of the order of $\eta_0 |\log \epsilon|$ for small $\eta_0 > 0$, with additional assumptions on σ_ϵ. However, the result as it is presented here suffices for our purposes.

Proof of Proposition 2.3.9. Thanks to (2.3.12) and (2.3.9) we can apply Proposition 2.3.7 to the function u_ϵ. We obtain two maps $w_\epsilon \in H^1(\partial B_1, \mathscr{N})$ and $\varphi^1_\epsilon \in H^1(B_1 \setminus B_{1-h(\epsilon)}, \mathbf{S}_0)$, which satisfy

$$\varphi^1_\epsilon(x) = u_\epsilon(x) \quad \text{and} \quad \varphi^1_\epsilon(x - h(\epsilon)x) = w_\epsilon(x) \qquad \text{for } \mathscr{H}^2\text{-a.e. } x \in \partial B_1,$$

$$\int_{\partial B_1} |\nabla w_\epsilon|^2 \, \mathrm{d}\mathscr{H}^2 \leq C,$$

$$E_\epsilon(\varphi^1_\epsilon, \, B_1 \setminus B_{1-h(\epsilon)}) \leq Ch(\epsilon). \tag{2.3.13}$$

Corollary 2.3.8, combined with (2.3.12), entails

$$\|w_\epsilon - v_\epsilon\|_{L^2(\partial B_1)} \leq \|w_\epsilon - u_\epsilon\|_{L^2(\partial B_1)} + \|u_\epsilon - v_\epsilon\|_{L^2(\partial B_1)} \leq C \left(h^{1/2}(\epsilon) + \sigma_\epsilon \right).$$

Therefore, setting $\tilde\sigma_\epsilon := h^{1/2}(\epsilon) + \sigma_\epsilon$, we have

$$\int_{\partial B_1} \left\{ |\nabla w_\epsilon|^2 + |\nabla v_\epsilon|^2 + \frac{|w_\epsilon - v_\epsilon|^2}{\tilde\sigma_\epsilon^2} \right\} \mathrm{d}\mathscr{H}^2 \leq C$$

Then, we can apply Lemma 2.3.6 to v_ϵ and w_ϵ, choosing $\sigma = \tilde{\sigma}_\epsilon$, $\beta = 3/4$ and $\lambda := \tilde{\sigma}_\epsilon^{1/4}$. By rescaling, we find a map $\varphi_\epsilon^2 \in H^1(B_{1-h(\epsilon)} \setminus B_{\nu_\epsilon}, \mathbf{S}_0)$ which satisfies

$$\int_{B_{1-h(\epsilon)}\setminus B_{\nu_\epsilon}} \left|\nabla\varphi_\epsilon^2\right|^2 \leq C\tilde{\sigma}_\epsilon^{1/4}\left(1-h(\epsilon)\right)$$

$$\operatorname{dist}(\varphi_\epsilon^2(x), \mathscr{N}) \leq C\tilde{\sigma}_\epsilon^{1/8} \qquad \text{for all } x \in B_{1-h(\epsilon)} \setminus B_{\nu_\epsilon}. \tag{2.3.14}$$

Since $\tilde{\sigma}_\epsilon \to 0$, there exists $\epsilon_1 > 0$ such that $\varphi_\epsilon^2(x) \notin \mathscr{C}$ for any $0 < \epsilon \leq \epsilon_1$ and x. Therefore, the function

$$\varphi_\epsilon(x) := \begin{cases} \varphi_\epsilon^1(x) & \text{if } x \in B_1 \setminus B_{1-h(\epsilon)} \\ \mathscr{R}(\varphi_\epsilon^2(x)) & \text{if } x \in B_{1-h(\epsilon)} \setminus B_{\nu_\epsilon} \end{cases}$$

is well-defined, belongs to $H^1(B_1 \setminus B_{\nu_\epsilon}, \mathscr{N})$, satisfies to (2.3.7) and

$$E_\epsilon(\varphi_\epsilon, B_1 \setminus B_{\nu_\epsilon}) = E_\epsilon(\varphi_\epsilon^1, B_1 \setminus B_{1-h(\epsilon)}) + \int_{B_{1-h(\epsilon)}\setminus B_{\nu_\epsilon}} \left|\nabla\varphi_\epsilon^2\right|^2 \overset{(2.3.13)\text{–}(2.3.14)}{\leq} C\nu_\epsilon. \qquad \square$$

Subsections 2.3.3–2.3.5 are devoted to the proof of Proposition 2.3.7, which we sketch here. From now on, we will assume that there exists a positive constant M such that

$$E_\epsilon(u_\epsilon, \partial B_1) \leq M\left|\log\epsilon\right| \qquad \text{for all } 0 < \epsilon < 1. \tag{M$_\epsilon$}$$

As in Luckhaus' arguments, the key ingredient of the construction is the choice of a grid on the unit sphere ∂B_1, with special properties. In Subsection 2.3.3 we construct a family of grids $\{\mathscr{G}^\epsilon\}$, whose cells have size controlled by $h(\epsilon) = \epsilon^{1/2}|\log\epsilon|$. Assuming that (M$_\epsilon$) holds, we prove that there exists $\epsilon_1 > 0$ such that

$$\operatorname{dist}(u_\epsilon(x), \mathscr{N}) \leq \delta_0 \qquad \text{for any } \epsilon \in (0, \epsilon_1) \text{ and any } x \in R_1^\epsilon.$$

Here R_1^ϵ denotes the 1-skeleton of $\mathscr{G}^\epsilon$, i.e. the union of all the 1-cells of $\mathscr{G}^\epsilon$. In particular, the composition $\mathscr{R} \circ u_\epsilon$ is well-defined on R_1^ϵ when $\epsilon \leq \epsilon_1$. It may or may not be possible to extend $\mathscr{R} \circ u_{\epsilon|R_1^\epsilon}$ to a map $v_\epsilon \colon \partial B_1 \to \mathscr{N}$ with controlled energy, depending on the homotopy properties of u_ϵ. A sufficient condition for the existence of v_ϵ is the following:

(C$_\epsilon$) For any 2-cell K of $\mathscr{G}^\epsilon$, the loop $\mathscr{R} \circ u_{\epsilon|\partial K} \colon \partial K \to \mathscr{N}$ is homotopically trivial.

This condition makes sense for any $u_\epsilon \in H^1(\partial B_1, \mathbf{S}_0)$. Indeed, we construct $\mathscr{G}^\epsilon$ in such a way that u_ϵ restricted to the 1-skeleton belongs to H^1. Then, by Sobolev injection, u_ϵ is continuous on the 1-skeleton.

In Subsection 2.3.4, we assume that (M$_\epsilon$) and (C$_\epsilon$) hold and we construct a function $v_\epsilon \in H^1(\partial B_1, \mathscr{N})$, whose energy is controlled by the energy of u_ϵ. Basically, we extend $\mathscr{R} \circ u_{\epsilon|\partial K}$ inside every 2-cell $K \in \mathscr{G}^\epsilon$, which is possible by Condition (C$_\epsilon$). Once v_ϵ is known, we construct φ_ϵ by Luckhaus' method. Particular care must be taken here, as we need to bound the potential energy of φ_ϵ as well.

Finally, in Subsection 2.3.5 we show that the logarithmic bound (2.3.8), for a small enough constant η_0, implies that Condition (C$_\epsilon$) is satisfied. Arguing by contra-position, we assume that (C$_\epsilon$) is not satisfied. Then, $\mathscr{R} \circ u_{\epsilon|\partial K}$ is non-trivial for at least one 2-cell $K \in \mathscr{G}^\epsilon$. In this case, using Jerrard-Sandier type lower bounds, we prove that the energy $E_\epsilon(u_\epsilon, \partial B_1)$ blows up at least as $\eta_1|\log\epsilon|$ for some $\eta_1 > 0$. Taking $\eta_0 < \eta_1$, this bound contradicts (2.3.8) and concludes the proof.

2.3.3 Good grids on the sphere

Consider a decomposition of ∂B_1 of the form

$$\partial B_1 = \bigcup_{j=0}^{2} \bigcup_{i=1}^{k_j} K_{i,j},$$

where the sets $K_{i,j}$ are mutually disjoint, and each $K_{i,j}$ is bilipschitz equivalent to a j-dimensional ball. The collection of all the $K_{i,j}$'s will be called a *grid* on ∂B_1. Each $K_{i,j}$ will be called a j-cell of the grid. We define the j-skeleton of the grid as

$$R_j := \bigcup_{i=1}^{k_j} K_{i,j} \qquad \text{for } j \in \{0,\, 1,\, 2\}.$$

For our purposes, we need to consider grids with some special properties.

Definition 2.3.1. Let $h\colon (0,\, \epsilon_1] \to (0,\, +\infty)$ be a fixed function. A *good family of grids* of size h is a family $\mathscr{G} := \{\mathscr{G}^\epsilon\}_{0<\epsilon\leq\epsilon_1}$ of grids on ∂B_1 which satisfies the following properties.

(G_1) There exists a constant $\Lambda > 0$ and, for each ϵ, i, j, a bilipschitz homeomorphism $\phi^\epsilon_{i,j}\colon K^\epsilon_{i,j} \to B^j_{h(\epsilon)}$ such that
$$\left\|\mathrm{D}\phi^\epsilon_{i,j}\right\|_{L^\infty} + \left\|\mathrm{D}(\phi^\epsilon_{i,j})^{-1}\right\|_{L^\infty} \leq \Lambda.$$

(G_2) For all $p \in \{1,\, 2,\, \ldots,\, k_1\}$ we have
$$\left|\left\{q \in \{1,\, 2,\, \ldots,\, k_2\}\colon K^\epsilon_{p,1} \subseteq K^\epsilon_{q,2}\right\}\right| \leq \Lambda,$$
i.e., each 1-cell is contained in the boundary of at most Λ 2-cells.

(G_3) We have
$$E_\epsilon(u_\epsilon,\, R^\epsilon_1) \leq Ch^{-1}(\epsilon)\, E_\epsilon(u_\epsilon,\, \partial B_1),$$
where R^ϵ_1 denotes the 1-skeleton of $\mathscr{G}^\epsilon$.

(G_4) There holds
$$\int_{R^\epsilon_1} f(u_\epsilon)\, \mathrm{d}\mathscr{H}^1 \leq Ch^{-1}(\epsilon) \int_{\partial B_1} f(u_\epsilon)\, \mathrm{d}\mathscr{H}^2.$$

Of course, this definition depends on the family $\{u_\epsilon\}$, which we assume to be fixed once and for all.

Lemma 2.3.10. *For any strictly positive function h, a good family of grids of size h exists.*

Proof. On the unit cube $\partial[0,\, 1]^3$, consider the uniform grid of size $\lceil h^{-1}(\epsilon)\rceil^{-1}$, i.e. the grid spanned by the points
$$\left(\lceil h^{-1}(\epsilon)\rceil^{-1}\mathbb{Z}^3\right) \cap \partial[0,\, 1]^3$$
(where $\lceil x\rceil$ is, by the definition, the smallest integer k such that $k \geq x$). By applying a bilipschitz homeomorphism $[0,\, 1]^3 \to \overline{B}_1$, one obtains a grid $\mathscr{F}^\epsilon$ on ∂B_1 which satisfy (G_1)–(G_2). Denote by T^ϵ_1 the 1-skeleton of $\mathscr{F}^\epsilon$. By an average argument, as in [92, Lemma 1], we find a rotation $\omega \in \mathrm{SO}(3)$ such that
$$E_\epsilon(u_\epsilon,\, \omega(T^\epsilon_1)) \leq Ch^{-1}(\epsilon)\, E_\epsilon(u_\epsilon,\, \partial B_1)$$
and
$$\int_{\omega(T^\epsilon_1)} f(u_\epsilon)\, \mathrm{d}\mathscr{H}^1 \leq Ch^{-1}(\epsilon) \int_{\partial B_1} f(u_\epsilon)\, \mathrm{d}\mathscr{H}^2.$$
Thus,
$$\mathscr{G}^\epsilon := \{\omega(K)\colon K \in \mathscr{F}^\epsilon\}$$
is a good family of grids of size h. $\square$

The interest of Definition 2.3.1 is explained by the following result.

Lemma 2.3.11. *Let $\mathscr{G}$ be a good family of grids on ∂B_1, of size h. Assume that there exists $\alpha \in (0, 1)$ such that*

$$\lim_{\epsilon \to 0} \epsilon^{-\alpha} h(\epsilon) = +\infty. \tag{2.3.15}$$

Then, there holds

$$\lim_{\epsilon \to 0} \sup_{x \in R_1^\epsilon} \operatorname{dist}(u_\epsilon(x), \mathscr{N}) = 0.$$

Proof. The arguments below are adapted from [2, Lemmas 3.4 and 3.10] (the reader is also referred to [17, Lemmas 2.2, 2.3 and 2.4]). Since the Landau-de Gennes potential satisfies (F_2) by Lemma 2.2.4, there exist positive numbers β, C and a continuous function $\psi\colon [0, +\infty) \to \mathbb{R}$ such that

$$\begin{cases} \psi(s) = \beta s^2 & \text{for } 0 \leq s < \delta_0 \\ 0 < \psi(s) \leq C & \text{for } s \geq \delta_0 \\ \psi(\operatorname{dist}(v, \mathscr{N})) \leq f(v) & \text{for any } v \in \mathbf{S}_0. \end{cases}$$

Denote by G a primitive of $\psi^{1/6}$, and set $d_\epsilon := \operatorname{dist}(u_\epsilon, \mathscr{N})$. Since the function $\operatorname{dist}(\cdot, \mathscr{N})$ is 1-Lipschitz continuous, we have $d_\epsilon \in H^1(\Omega, \mathbb{R})$ and $|\nabla d_\epsilon| \leq |\nabla u_\epsilon|$. Moreover, $\psi(d_\epsilon) \leq f(u_\epsilon)$ by construction of ψ. Thus, (M_ϵ) and (G_3) entail

$$C\left|\log \epsilon\right| \geq h(\epsilon) \int_{R_1^\epsilon} \left\{ \frac{1}{2} \left|\nabla d_\epsilon\right|^2 + \epsilon^{-2} \psi(d_\epsilon) \right\} \mathrm{d}\mathscr{H}^1$$

By applying Young's inequality $a + b \geq C a^{3/4} b^{1/4}$, we obtain

$$\begin{aligned} C\left|\log \epsilon\right| &\geq C\epsilon^{-1/2} h(\epsilon) \int_{R_1^\epsilon} \left|\nabla d_\epsilon\right|^{3/2} \psi^{1/4}(d_\epsilon) \,\mathrm{d}\mathscr{H}^1 \\ &= C\epsilon^{-1/2} h(\epsilon) \int_{R_1^\epsilon} \left|\nabla G(d_\epsilon)\right|^{3/2} \,\mathrm{d}\mathscr{H}^1. \end{aligned} \tag{2.3.16}$$

Fix a 1-cell K of $\mathscr{G}_\epsilon$. With the Sobolev-Morrey embedding $W^{1,3/2}(K) \hookrightarrow C^0(K)$ and (2.3.16), we can control the oscillations of $G(d_\epsilon)$ over K:

$$\begin{aligned} \left(\operatorname*{osc}_K G(d_\epsilon)\right)^{3/2} &\leq C h^{1/2}(\epsilon) \int_K \left|\nabla G(d_\epsilon)\right|^{3/2} \,\mathrm{d}\mathscr{H}^1 \\ &= C \epsilon^{1/2} h^{-1/2}(\epsilon) \left|\log \epsilon\right|. \end{aligned}$$

A factor $h^{1/2}(\epsilon)$ appears in the right-hand side of this inequality, due to scaling. In view of (2.3.15), we obtain

$$\operatorname*{osc}_{R_1^\epsilon} G(d_\epsilon) \to 0$$

as $\epsilon \to 0$. But G is a continuous and strictly increasing function, so G has a continuous inverse. This implies

$$\operatorname*{osc}_{R_1^\epsilon} d_\epsilon \to 0 \tag{2.3.17}$$

as $\epsilon \to 0$. On the other hand, (M_ϵ), (G_3) and (2.3.15) yield

$$⨍_K \psi(d_\epsilon) \,\mathrm{d}\mathscr{H}^1 \leq \frac{1}{h(\epsilon)} \int_{R_1^\epsilon} f(u_\epsilon) \,\mathrm{d}\mathscr{H}^1 \leq C \epsilon^2 h^{-1}(\epsilon) \left|\log \epsilon\right| \to 0 \tag{2.3.18}$$

as $\epsilon \to 0$, for any 1-cell K of $\mathscr{G}_\epsilon$. As we will see in a moment, this implies

$$\sup_K ⨍_K d_\epsilon \,\mathrm{d}\mathscr{H}^1 \to 0. \tag{2.3.19}$$

Therefore, combining (2.3.19) with (2.3.17), we conclude that d_ϵ converges uniformly to 0 as $\epsilon \to 0$.

Now, we check that (2.3.19) holds. There exists a constant $\kappa > 0$ such that

$$\|d_\epsilon\|_{L^\infty(\Omega)} \leq \kappa$$

(this follows from the uniform L^∞ estimate for u_ϵ (2.3.9)). For any $\delta \in (0, \kappa)$, set

$$\psi_*(\delta) := \inf_{\delta \leq s \leq \kappa} \psi(s) > 0.$$

Then,

$$\frac{\mathscr{H}^1(\{d_\epsilon \geq \delta\} \cap K)}{\mathscr{H}^1(K)} \psi_*(\delta) \leq \frac{1}{\mathscr{H}^1(K)} \int_{\{d_\epsilon \geq \delta\} \cap K} \psi(d_\epsilon) \, \mathrm{d}\mathscr{H}^1 \leq \fint_K \psi(d_\epsilon) \, \mathrm{d}\mathscr{H}^1. \tag{2.3.20}$$

Thus, for any 1-cell K, we have

$$\begin{aligned} 0 \leq \fint_K d_\epsilon \, \mathrm{d}\mathscr{H}^1 &= \frac{1}{\mathscr{H}^1(K)} \int_{\{d_\epsilon \leq \delta\} \cap K} d_\epsilon \, \mathrm{d}\mathscr{H}^1 + \frac{1}{\mathscr{H}^1(K)} \int_{\{d_\epsilon \geq \delta\} \cap K} d_\epsilon \, \mathrm{d}\mathscr{H}^1 \\ &\leq \frac{\mathscr{H}^1(\{d_\epsilon \leq \delta\} \cap K)}{\mathscr{H}^1(K)} \delta + \frac{\mathscr{H}^1(\{d_\epsilon \geq \delta\} \cap K)}{\mathscr{H}^1(K)} \kappa \\ &\overset{(2.3.20)}{\leq} \delta + \frac{\kappa}{\psi_*(\delta)} \fint_K \psi(d_\epsilon) \, \mathrm{d}\mathscr{H}^1 \\ &\overset{(2.3.18)}{\leq} \delta + \frac{C\kappa}{\psi_*(\delta)} \epsilon^2 h^{-1}(\epsilon) \, |\log \epsilon| \, . \end{aligned}$$

We pass to the limit first as $\epsilon \to 0$, then as $\delta \to 0$. Using (2.3.15), we deduce (2.3.19). □

2.3.4 Construction of v_ϵ and φ_ϵ

First, we construct the approximating map $v_\epsilon \colon \partial B_1 \to \mathscr{N}$.

Lemma 2.3.12. *Assume that* (M_ϵ), (C_ϵ) *hold. There exists $\epsilon_1 > 0$ such that, for any $0 < \epsilon \leq \epsilon_1$, there exists a map $v_\epsilon \in H^1(\partial B_1, \mathscr{N})$ which satisfy* (2.3.10),

$$v_\epsilon(x) = \mathscr{R}(u_\epsilon(x)) \qquad \text{and} \qquad |u_\epsilon(x) - v_\epsilon(x)| \leq \delta_0 \tag{2.3.21}$$

for every $x \in R_1^\epsilon$.

Proof. To construct v_ϵ, we take a family $\mathscr{G} = \{\mathscr{G}^\epsilon\}_{\epsilon > 0}$ of grids of size

$$h(\epsilon) := \epsilon^{1/2} \, |\log \epsilon| \tag{2.3.22}$$

(such a family exists by Lemma 2.3.10). Condition (2.3.15) is satisfied for $\alpha = 1/2$, so by Lemma 2.3.11 there exists $\epsilon_1 > 0$ such that

$$\mathrm{dist}(u_\epsilon(x), \mathscr{N}) \leq \delta_0 \qquad \text{for any } \epsilon \in (0, \epsilon_1) \text{ and any } x \in R_1^\epsilon.$$

In particular, the formula

$$v_\epsilon(x) := \mathscr{R}(u_\epsilon(x)) \qquad \text{for all } x \in R_1^\epsilon$$

defines a function $v_\epsilon \in H^1(R_1^\epsilon, \mathbf{S}_0)$, which satisfies (2.3.21).

To extend v_ϵ inside each 2-cell, we take advantage of Lemma 2.3.2. Fix a 2-cell K of the grid $\mathscr{G}_\epsilon$. Since we assume that Condition (C_ϵ) holds, $v_{\epsilon|\partial K}$ is homotopically trivial and it can be extended to a map $g_{\varepsilon,K} \in H^1(K, \mathscr{N})$. Therefore, with the help of (G$_1$) and Lemma 2.3.2 we find $v_{\epsilon,K} \in H^1(K, \mathscr{N})$ such that $v_{\epsilon,K|\partial K} = v_{\epsilon|\partial K}$ and

$$\int_K |\nabla v_{\epsilon,K}|^2 \, \mathrm{d}\mathscr{H}^2 \leq Ch(\epsilon) \int_{\partial K} |\nabla v_\epsilon|^2 \, \mathrm{d}\mathscr{H}^1.$$

Define $v_\epsilon \colon \partial B_1 \to \mathscr{N}$ by setting $v_\epsilon := v_{\epsilon,K}$ on each 2-cell K. This function agrees with $v_{\epsilon|R^1_\epsilon}$ previously defined by (2.3.21), hence the notation is not ambiguous. Moreover, $v_\epsilon \in H^1(\partial B_1, \mathscr{N})$ and

$$\begin{aligned} \int_{\partial B_1} |\nabla v_\epsilon|^2 \, \mathrm{d}\mathscr{H}^2 &\leq \sum_K \int_K |\nabla v_\epsilon|^2 \, \mathrm{d}\mathscr{H}^2 \leq Ch(\epsilon) \sum_K \int_{\partial K} |\nabla v_\epsilon|^2 \, \mathrm{d}\mathscr{H}^1 \\ &\overset{(G_2)}{\leq} Ch(\epsilon) \int_{R_1^\epsilon} |\nabla v_\epsilon|^2 \, \mathrm{d}\mathscr{H}^1 \overset{(2.3.21)}{\leq} Ch(\epsilon) \int_{R_1^\epsilon} |\nabla u_\epsilon|^2 \, \mathrm{d}\mathscr{H}^1 \\ &\overset{(G_3)}{\leq} CE_\epsilon(u_\epsilon, \partial B_1), \end{aligned}$$

where the sum runs over all the 2-cells K of $\mathscr{G}_\epsilon$. Thus, we have constructed a function v_ϵ which satisfies (2.3.10) and (2.3.21), so Lemma 2.3.12 is proved. □

Now, we construct the interpolation map $\varphi_\epsilon \colon \partial B_1 \to \mathbf{S}_0$.

Lemma 2.3.13. *Assume that the conditions* (M$_\epsilon$), (C$_\epsilon$) *are fulfilled. Then, for any* $0 < \epsilon \leq \epsilon_1$ *there exists a map* $\varphi_\epsilon \in H^1(B_1 \setminus B_{1-h(\epsilon)}, \mathbf{S}_0)$ *which satisfy* (2.3.7) *and* (2.3.11).

Proof. For the sake of simplicity, set $A_\epsilon := B_1 \setminus B_{1-h(\epsilon)}$. The grid $\mathscr{G}^\epsilon$ on ∂B_1 induces a grid $\hat{\mathscr{G}}^\epsilon$ on A_ϵ, whose cells are

$$\hat{K} := \left\{ x \in \mathbb{R}^3 \colon 1 - h(\epsilon) \leq |x| \leq 1, \, \frac{x}{|x|} \in K \right\} \qquad \text{for each } K \in \mathscr{G}^\epsilon.$$

If K is a cell of dimension j, then $\hat{K}$ has dimension $j+1$. For $j \in \{0, 1, 2\}$, we call $\hat{R}^\epsilon_j$ the union of all the $(j+1)$-cells of $\hat{\mathscr{G}}^\epsilon$.

The function φ_ϵ is constructed as follows. If $x \in \partial B_1 \cup \partial B_{1-h(\epsilon)}$, then $\varphi_\varepsilon(x)$ is determined by (2.3.7). If $x \in \hat{R}^\epsilon_1 \cup \hat{R}^\epsilon_1$, we define $\varphi_\epsilon(x)$ by linear interpolation:

$$\varphi_\epsilon(x) := \frac{1 - |x|}{h(\epsilon)} \, u_\epsilon\left(\frac{x}{|x|}\right) + \frac{h(\epsilon) - 1 + |x|}{h(\epsilon)} \, v_\epsilon\left(\frac{x}{|x|}\right). \tag{2.3.23}$$

For any 3-cell $\hat{K}$ of $\mathscr{G}_\epsilon$, we extend homogeneously (of degree 0) the function $\varphi_{\epsilon|\partial\hat{K}}$ on $\hat{K}$. This gives a map $\varphi_\epsilon \in H^1(\hat{K})$, because $\hat{K}$ is a cell of dimension 3. As a result, we obtain a map $\varphi_\epsilon \in H^1(A_\epsilon, \mathbf{S}_0)$ which satisfies (2.3.7).

To complete the proof of the lemma, we only need to bound the energy of φ_ϵ on A_ϵ. Since φ_ϵ has been obtained by homogeneous extension on cells of size $h(\epsilon)$, we have

$$\begin{aligned} E_\epsilon(\varphi_\epsilon, A_\epsilon) &\overset{(G_1)}{\leq} Ch(\epsilon) \sum_{\hat{K}} E_\epsilon(\varphi_\epsilon, \partial\hat{K}) \\ &\overset{(G_2)}{\leq} Ch(\epsilon) \Big\{ E_\epsilon(u_\epsilon, \partial B_1) + E_\epsilon(v_\epsilon, \partial B_{1-h(\epsilon)}) + E_\epsilon(\varphi_\epsilon, \hat{R}^\epsilon_1) \Big\}, \end{aligned} \tag{2.3.24}$$

where the sum runs over all the 3-cells $\hat{K}$ of $\hat{\mathscr{G}}^\epsilon$. To conclude the proof, we invoke the following fact.

Lemma 2.3.14. *We have*

$$E_\epsilon(\varphi_\epsilon, \hat{R}^\epsilon_1) \leq C \left(\epsilon^2 h^{-2}(\epsilon) + 1\right) E_\epsilon(u_\epsilon, \partial B_1).$$

From (2.3.24) and Lemma 2.3.14 we get

$$E_\epsilon(\varphi_\epsilon,\, A_\epsilon) \le Ch(\epsilon)\Big\{ \left(\epsilon^2 h^{-2}(\epsilon)+1\right) E_\epsilon(u_\epsilon,\, \partial B_1) + E_\epsilon(v_\epsilon,\, \partial B_{1-h(\epsilon)})\Big\}$$
$$\stackrel{(2.3.10)}{\le} Ch(\epsilon)\left(\epsilon^2 h^{-2}(\epsilon)+1\right) E_\epsilon(u_\epsilon,\, \partial B_1)$$

and, thanks to our choice (2.3.22) of $h(\epsilon)$, we conclude that (2.3.11) holds, so Lemma 2.3.13 is proved. □

Proof of Lemma 2.3.14. We consider first the contribution of the potential energy. Thanks to (F_3), (2.3.23) and (2.3.21), we deduce that

$$f(\varphi_\epsilon(x)) \le C\left(\frac{1-|x|}{h(\epsilon)}\right)^2 f\left(u_\epsilon\left(\frac{x}{|x|}\right)\right) \qquad \text{for } x \in \hat{R}_1^\epsilon.$$

By integration, this gives

$$\int_{\hat{R}_1^\epsilon} f(\varphi_\epsilon)\,\mathrm{d}\mathscr{H}^2 \le Ch(\epsilon)\int_{R_1^\epsilon} f(u_\epsilon)\,\mathrm{d}\mathscr{H}^2. \tag{2.3.25}$$

Now, we turn to the elastic part of the energy. Using again the definition (2.3.23) of φ_ϵ on $\hat{R}_1^\epsilon$, we have

$$\int_{\hat{R}_1^\epsilon} |\nabla\varphi_\epsilon|^2\,\mathrm{d}\mathscr{H}^2 \le Ch^{-1}(\epsilon)\int_{R_1^\epsilon} |u_\epsilon - v_\epsilon|^2\,\mathrm{d}\mathscr{H}^1. \tag{2.3.26}$$

The condition (F_2) on the Landau-de Gennes potential, together with (2.3.21), implies

$$\int_{R_1^\epsilon} |u_\epsilon - v_\epsilon|^2\,\mathrm{d}\mathscr{H}^1 \le C\int_{R_1^\epsilon} f(u_\epsilon)\,\mathrm{d}\mathscr{H}^1. \tag{2.3.27}$$

Using (2.3.25), (2.3.26) and (2.3.27), we deduce that

$$E_\epsilon(\varphi_\epsilon, \hat{R}_1^\epsilon) \le C\left(h^{-1}(\epsilon) + \epsilon^{-2}h(\epsilon)\right)\int_{R_1^\epsilon} f(u_\epsilon)\,\mathrm{d}\mathscr{H}^1.$$

Because of Condition (G_4) in the definition of a good grid, we obtain

$$E_\epsilon(\varphi_\epsilon, \hat{R}_1^\epsilon) \le C\left(h^{-2}(\epsilon) + \epsilon^{-2}\right)\int_{\partial B_1} f(u_\epsilon)\,\mathrm{d}\mathscr{H}^2$$

so the lemma follows easily. □

2.3.5 Logarithmic bounds for the energy imply (C_ϵ)

Aim of this subsection is to establish the following lemma, and conclude the proof of Proposition 2.3.7.

Lemma 2.3.15. *There exists $\eta_1 = \eta_1(\mathscr{N},\, \Lambda,\, M,\, \epsilon_1)$ such that, if $0 < \epsilon \le \epsilon_1$ and u_ϵ satisfies* (M_ϵ), (2.3.9) *but* not (C_ϵ)*, then*

$$E_\epsilon(u_\epsilon,\, \partial B_1) \ge \eta_1 \left|\log\epsilon\right|.$$

Once Lemma 2.3.15 is proved, Proposition 2.3.7 follows in an elementary way.

Proof of Proposition 2.3.7. Choose $\eta_0 := \eta_1/2$. If u_ϵ satisfies (2.3.8) with this choice of η_0 and (2.3.9), then it must satisfy Condition (C_ϵ), otherwise Lemma 2.3.15 would yield a contradiction. Then, the proposition follows by Lemmas 2.3.12 and 2.3.13. □

Proof of Lemma 2.3.15. By assumption, Condition (C_ϵ) is not satisfied, so there exists a 2-cell $K^* \in \mathscr{G}^\epsilon$ such that $\mathscr{R} \circ u_{\epsilon|\partial K^*}$ is non-trivial. By Definition 2.3.1, there exists a bilipschitz homeomorphism $\phi\colon K_* \to B_{h(\epsilon)}$ which satisfies (G_1). Therefore, up to composition with ϕ we can assume that K_* is a 2-dimensional disk, $K_* = B^2_{h(\epsilon)}$. Lemma 2.3.11 implies that $u_\epsilon(x) \notin \mathscr{C}_0$ for every $x \in \partial K_*$, for $0 < \epsilon \leq \epsilon_1$. Thanks to this fact and to (2.3.9) we can apply Corollary 2.2.6, and we deduce

$$E_\epsilon(u_\epsilon,\, K_*) + Ch(\epsilon)E_\epsilon(u_\epsilon,\, \partial K_*) \geq \kappa_* \log \frac{h(\epsilon)}{\epsilon} - C$$

On the other hand, condition (G_3) yields

$$E_\epsilon(u_\epsilon,\, K_*) + Ch(\epsilon)E_\epsilon(u_\epsilon,\, \partial K_*) \leq CE_\epsilon(u_\epsilon,\, \partial B_1).$$

Due to the previous inequalities and (2.3.22), we infer

$$E_\epsilon(u_\epsilon,\, \partial B_1) \geq C\left\{\log\left(\epsilon^{-1/2}\left|\log \epsilon\right|\right) - 1\right\} \geq C\left(\frac{1}{2}\left|\log\epsilon\right| - 1\right)$$

for all $0 < \epsilon \leq \epsilon_1 < 1$, so the lemma follows. □

2.4 The asymptotic analysis of Landau-de Gennes minimizers

2.4.1 Concentration of the energy: Proof of Proposition 2.1.6

This whole section aims at proving Theorem 2.1.1. Let η_0, ϵ_1 be given by Proposition 2.3.7, and set $\epsilon_0 := \epsilon_1\theta$. Throughout the section, the same symbol C will be used to denote several different constants, possibly depending on θ and ϵ_0, but not on ε, R. To simplify the notation, from now on we assume that $x_0 = 0$. For a fixed $0 < \varepsilon \leq \epsilon_0 R$, define the set

$$D^\varepsilon := \left\{r \in (\theta R,\, R)\colon E_\varepsilon(Q_\varepsilon,\, \partial B_r) \leq \frac{2\eta}{1-\theta}\log\frac{R}{\varepsilon}\right\}.$$

The elements of D^ε are the "good radii", i.e. $r \in D^\varepsilon$ means that we have a control on the energy on the sphere of radius r. Assume that the condition (2.1.10) is satisfied. Then, by an average argument we deduce that

$$\mathscr{H}^1(D^\varepsilon) \geq \frac{(1-\theta)R}{2}. \tag{2.4.1}$$

For any $r \in D^\varepsilon$ we have

$$E_\varepsilon(Q_\varepsilon,\, \partial B_r) \leq \frac{2\eta}{1-\theta}\left(\log\frac{r}{\varepsilon} - \log\theta\right),$$

since $R \leq \theta^{-1}r$. By choosing η small enough, we can assume that

$$E_\varepsilon(Q_\varepsilon,\, \partial B_r) \leq \eta_0 \log\frac{r}{\varepsilon} \qquad \text{for any } r \in D^\varepsilon \text{ and } 0 < \varepsilon \leq \epsilon_0 R. \tag{2.4.2}$$

In particular, our choice of η depends on ϵ_1, η_0, θ.

Lemma 2.4.1. *For any $0 < \varepsilon \leq \epsilon_0 R$ and any $r \in D^\varepsilon$, there holds*

$$E_\varepsilon(Q_\varepsilon,\, B_r) \leq CR\left(E_\varepsilon^{1/2}(Q_\varepsilon,\, \partial B_r) + 1\right).$$

A similar inequality was obtained by Hardt, Kinderlehrer and Lin in [60, Lemma 2.3, Equation (2.3)], and it played a crucial role in the proof of their energy improvement result.

Proof of Lemma 2.4.1. To simplify the notations, we get rid of r by means of a scaling argument. Set $\epsilon := \varepsilon/r$, and define the function $u_\epsilon\colon B_1 \to \mathbf{S}_0$ by

$$u_\epsilon(x) := Q_\varepsilon(rx) \qquad \text{for all } x \in B_1.$$

The lemma will be proved once we show that

$$E_\epsilon(u_\epsilon,\, B_1) \leq C E_\epsilon^{1/2}(u_\epsilon,\, \partial B_1) + 1 \tag{2.4.3}$$

(multiplying both sides of (2.4.3) by r and using that $r \leq R$ yields the lemma). Since we have assumed that $r \in D^\varepsilon$ we have, by scaling of (2.4.2),

$$E_\epsilon(u_\epsilon,\, \partial B_1) \leq \eta_0 \left|\log \epsilon\right|.$$

Moreover, u_ϵ satisfies the $W^{1,\infty}$-bound (2.3.9), due to Lemma 2.2.11. Therefore, we can apply Proposition 2.3.7 and find $v_\epsilon \in H^1(\partial B_1,\, \mathscr{N})$, $\varphi_\epsilon \in H^1(A_\epsilon,\, \mathbf{S}_0)$ which satisfy

$$\varphi_\epsilon(x) = u_\epsilon(x) \quad \text{and} \quad \varphi_\epsilon(x - h(\epsilon)x) = v_\epsilon(x) \qquad \text{for } \mathscr{H}^2\text{-a.e. } x \in \partial B_1$$

$$\int_{\partial B_1} \left|\nabla v_\epsilon\right|^2 \mathrm{d}\mathscr{H}^2 \leq C E_\epsilon(u_\epsilon,\, \partial B_1), \tag{2.4.4}$$

$$E_\epsilon(\varphi_\epsilon,\, A_\epsilon) \leq C h(\epsilon) E_\epsilon(u_\epsilon,\, \partial B_1). \tag{2.4.5}$$

Here $h(\epsilon) := \epsilon^{1/2}|\log \epsilon|$ and $A_\epsilon := B_1 \setminus B_{1-h(\epsilon)}$. By applying Lemma 2.3.1 to v_ϵ, we find a map $w_\epsilon \in H^1(B_1,\, \mathscr{N})$ such that $w_{\epsilon|\partial B_1}$ and

$$\int_{B_1} \left|\nabla w_\epsilon\right|^2 \leq C \left\{ \int_{\partial B_1} \left|\nabla v_\epsilon\right|^2 \mathrm{d}\mathscr{H}^2 \right\}^{1/2} \overset{(2.4.4)}{\leq} C E_\epsilon^{1/2}(u_\epsilon,\, \partial B_1). \tag{2.4.6}$$

Now, define the function $\tilde{w}_\epsilon\colon B_1 \to \mathbf{S}_0$ by

$$\tilde{w}_\epsilon(x) := \begin{cases} \varphi_\epsilon(x) & \text{for } x \in A_\epsilon \\ w_\epsilon\left(\dfrac{x}{1-h(\epsilon)}\right) & \text{for } x \in B_{1-h(\epsilon)}. \end{cases}$$

The energy of $\tilde{w}_\epsilon$ in the spherical shell A_ϵ is controlled by (2.4.5). Due to our choice of the parameter $h(\epsilon)$, we deduce that

$$E_\epsilon(\tilde{w}_\epsilon,\, A_\epsilon) \leq 1,$$

provided that ε_0 is small enough. Combining this with (2.4.6), we obtain

$$E_\epsilon(\tilde{w}_\epsilon,\, B_1) \leq C E_\epsilon^{1/2}(u_\epsilon,\, \partial B_1) + 1.$$

But $\tilde{w}_\epsilon$ is an admissible comparison function for u_ϵ on B_1, because $\tilde{w}_\epsilon = u_\epsilon$ on ∂B_1. Thus, the minimality of u_ϵ implies (2.4.3). □

Lemma 2.4.1 can be seen as a non-linear differential inequality for the function $y\colon r \in (\theta R,\, R) \mapsto E_\varepsilon(Q, B_r)$. The conclusion of the proof of Proposition 2.1.6 follows now by a simple ODE argument.

Lemma 2.4.2. *Let α, β be two positive numbers. Let $y \in W^{1,1}([r_0,\, r_1],\, \mathbb{R})$ be a function such that $y' \geq 0$ a.e., and let $D \subseteq (r_0,\, r_1)$ be a measurable set such that $\mathscr{H}^1(D) \geq (r_1 - r_0)/2$. If the function y satisfies*

$$y(r) \leq \alpha y'(r)^{1/2} + \beta \qquad \text{for } \mathscr{H}^1\text{-a.e. } r \in D, \tag{2.4.7}$$

then there holds

$$y(r_0) \leq \beta + \frac{2\alpha^2}{r_1 - r_0}.$$

Proof. If there exists a point $r_* \in (r_0, r_1)$ such that $y(r_*) \leq \beta$, then $y(r_0) \leq \beta$ (because y is an increasing function) and the lemma is proved. Therefore, we can assume without loss of generality that $y - \beta > 0$ on (r_0, r_1). Then, Equation (2.4.7) and the monotonicity of y imply

$$\frac{y'(r)}{(y(r)-\beta)^2} \geq \alpha^{-2}\mathbb{1}_D(r) \qquad \text{for a.e. } r \in (r_0, r_1)$$

where $\mathbb{1}_D$ is the characteristic function of D (that is, $\mathbb{1}_D(r) = 1$ if $r \in D$ and $\mathbb{1}_D(r) = 0$ otherwise). By integrating this inequality on $(0, r)$, we deduce

$$\frac{1}{y(r_0)-\beta} - \frac{1}{y(r)-\beta} \geq \alpha^{-2}\mathscr{H}^1\left((r_0, r)\cap D\right) \qquad \text{for any } r \in (r_0, r_1).$$

Since we have assumed that $\mathscr{H}^1(D) \geq (r_1 - r_0)/2$, we obtain

$$\mathscr{H}^1((r_0, r)\cap D) \geq \left(r - \frac{r_0+r_1}{2}\right)^+ := \max\left\{r - \frac{r_0+r_1}{2}, 0\right\}$$

so, via an algebraic manipulation,

$$y(r) \geq \beta + \frac{y(r_0)-\beta}{1-\alpha^{-2}\left(r-(r_0+r_1)/2\right)^+(y(r_0)-\beta)} \qquad \text{for any } r \in (r_0, r_1).$$

Since y is well-defined (and finite) up to $r = r_1$, there must be

$$1 - \frac{r_1-r_0}{2\alpha^2}\left(y(r_0)-\beta\right) > 0,$$

whence the lemma follows. □

Conclusion of the proof of Proposition 2.1.6. Thanks to Lemma 2.4.1 and (2.4.1), we can apply Lemma 2.4.2 to the function $y(r) := E_\varepsilon(Q_\varepsilon, B_r)$, for $r \in (\theta R, R)$, and the set $D := D^\varepsilon$. This yields

$$E_\varepsilon(Q_\varepsilon, B_{\theta R}) \leq CR,$$

so the proposition is proved. □

2.4.2 Interior energy bounds imply convergence to a harmonic map

In this subsection, we suppose that minimizers satisfy

$$E_\varepsilon(Q_\varepsilon, B_R(x_0)) \leq CR \tag{2.4.8}$$

on a ball $B_r(x_0) \subset\subset \Omega$. In interesting situations, where line defects appear, such an estimate is not valid over the whole of the domain. However, (2.4.8) is satisfied locally, away from a singular set. The main result of this subsection is the following:

Proposition 2.4.3. *Assume that $\overline{B}_R(x_0) \subseteq \Omega$ and that* (2.4.8) *is satisfied for some positive constants R, C. Fix $0 < \theta < 1$. Then, there exist a subsequence $\varepsilon_n \searrow 0$ and a map $Q_0 \in H^1(B_{\theta R}(x_0), \mathscr{N})$ such that*

$$Q_{\varepsilon_n} \to Q_0 \qquad \textit{strongly in } H^1(B_{\theta R}(x_0), \mathbf{S}_0).$$

The map Q_0 is minimizing harmonic on $B_{\theta R}(x_0)$, that is, for any $Q \in H^1(B_{\theta R}(x_0), \mathscr{N})$ such that $Q = Q_0$ on $\partial B_{\theta R}(x_0)$ there holds

$$\frac{1}{2}\int_{B_{\theta R}(x_0)} |\nabla Q_0|^2 \leq \frac{1}{2}\int_{B_{\theta R}(x_0)} |\nabla Q|^2 .$$

In general, we cannot expect the map Q_0 to be smooth (an example was given in Section 2.1). In contrast, by Schoen and Uhlenbeck's partial regularity result [125, Theorem II] we know that there exists a finite set $\mathscr{S}_{\mathrm{pts}} \subseteq B_{\theta R}(x_0)$ such that Q_0 is smooth on $B_{\theta R}(x_0) \setminus \mathscr{S}_{\mathrm{pts}}$. Accordingly, the sequence $\{Q_{\varepsilon_n}\}$ will not converge uniformly to Q_0 on the whole of $B_{\theta R}(x_0)$, in general, but we can prove the uniform convergence away from the singularities of Q_0.

Proposition 2.4.4. *Let $K \subseteq B_{\theta R}(x_0)$ be such that Q_0 is smooth on the closure of K. Then $Q_{\varepsilon_n} \to Q_0$ uniformly on K.*

The asymptotic behaviour of minimizers of the Landau-de Gennes functional, in the bounded-energy regime (2.4.8), was already studied by Majumdar and Zarnescu in [98]. In that paper, H^1-convergence to a harmonic map and local uniform convergence away from the singularities of Q_0 were already proven. However, in our case some extra care must be taken, because of the local nature of our assumption (2.4.8).

Proof of Proposition 2.4.3. Up to a translation, we assume that $x_0 = 0$. In view of (2.4.8), there exists a subsequence $\varepsilon_n \searrow 0$ and a map $Q_0 \in H^1(B_R, \mathbf{S}_0)$ such that

$$Q_{\varepsilon_n} \to Q_0 \qquad \text{weakly in } H^1(B_R, \mathbf{S}_0), \text{ strongly in } L^2(B_R, \mathbf{S}_0) \text{ and a.e.}$$

Using Fatou's lemma and (2.4.8) again, we also see that

$$\int_{B_R} f(Q_0) \leq \liminf_{n\to+\infty} \varepsilon_n^2 E_{\varepsilon_n}(Q_{\varepsilon_n}, B_R) \leq \liminf_{n\to+\infty} \varepsilon_n^2 CR = 0,$$

hence $f(Q_0) = 0$ a.e. or, equivalently,

$$Q_0(x) \in \mathscr{N} \qquad \text{for a.e. } x \in B_1.$$

By means of a comparison argument, we will prove that Q_{ε_n}'s actually converge *strongly* in H^1. Fatou's lemma combined with (2.4.8) gives

$$\int_{\theta R}^{R} \liminf_{n\to+\infty} E_{\varepsilon_n}(Q_{\varepsilon_n}, \partial B_r)\,\mathrm{d}r \leq \liminf_{n\to+\infty} E_{\varepsilon_n}(Q_{\varepsilon_n}, B_R \setminus B_{\theta R}) \leq CR. \tag{2.4.9}$$

Therefore, the set

$$\left\{ r \in (0, R] \colon \liminf_{n\to+\infty} E_{\varepsilon_n}(Q_{\varepsilon_n}, \partial B_r) > \frac{2C}{1-\theta} \right\}$$

must have length $\leq (1-\theta)R/2$, otherwise (2.4.9) would be violated. In particular, there exist a radius $r \in (\theta R, R]$ and a relabeled subsequence such that

$$E_{\varepsilon_n}(Q_{\varepsilon_n}, \partial B_r) \leq \frac{2C}{1-\theta}.$$

For ease of notation we scale the variables, setting $\epsilon_n := \varepsilon_n / r$,

$$u_n(x) := Q_{\varepsilon_n}(rx) \qquad \text{and} \qquad u_*(x) := Q_0(rx) \qquad \text{for } x \in B_1.$$

The scaled maps satisfy

$$u_n \to u_* \qquad \text{weakly in } H^1(B_1, \mathbf{S}_0), \text{ strongly in } L^2(B_1, \mathbf{S}_0) \text{ and a.e.,} \tag{2.4.10}$$

$$u_*(x) \in \mathscr{N} \qquad \text{for a.e. } x \in B_1, \tag{2.4.11}$$

$$E_{\epsilon_n}(u_n, \partial B_1) \leq C. \tag{2.4.12}$$

By (2.4.10) and the trace theorem, $u_n \rightharpoonup u_*$ weakly in $H^{1/2}(\partial B_1, \mathbf{S}_0)$ and hence, by compact embedding, strongly in $L^2(\partial B_1, \mathbf{S}_0)$. Moreover, by (2.4.12) $u_n \rightharpoonup u_*$ weakly in $H^1(\partial B_1, \mathbf{S}_0)$, so

$$\frac{1}{2}\int_{\partial B_1} |\nabla u_*|^2 \,\mathrm{d}\mathscr{H}^2 \leq \limsup_{n\to+\infty} E_{\epsilon_n}(u_n, \partial B_r) \leq C. \tag{2.4.13}$$

We are going to apply Proposition 2.3.9 to interpolate between u_n and u_*. Set $\sigma_n := \|u_n - u_*\|_{L^2(\partial B_1)}$. Then $\sigma_n \to 0$ and

$$\int_{\partial B_1} \left\{ |\nabla u_n|^2 + \frac{1}{\epsilon_n} f(u_n) + |\nabla u_*|^2 + \frac{|u_n - u_*|^2}{\sigma_n} \right\} \mathrm{d}\mathscr{H}^2 \leq C,$$

because of (2.4.12), (2.4.13). Moreover, the $W^{1,\infty}$-estimate (2.3.9) is satisfied by Lemma 2.2.11. Thus, Proposition 2.3.9 applies. We find a positive sequence $\nu_n \to 0$ and functions $\varphi_n \in H^1(B_1 \setminus B_{1-\nu_n}, \mathbf{S}_0)$ which satisfy

$$\varphi_n(x) = u_n(x), \qquad \varphi_n(x - \nu_n x) = u_*(x)$$

for $\mathscr{H}^2$-a.e. $x \in \partial B_1$ and

$$E_{\epsilon_n}(\varphi_n, B_1 \setminus B_{1-\nu_n}) \leq C\nu_n. \tag{2.4.14}$$

Now, let $w_* \in H^1(B_1, \mathscr{N})$ be a minimizing harmonic extension of $u_{*|\partial B_1}$, i.e.

$$\frac{1}{2}\int_{B_1} |\nabla w_*|^2 \leq \frac{1}{2}\int_{B_1} |\nabla w|^2 \tag{2.4.15}$$

for any $w \in H^1(B_1, \mathscr{N})$ such that $w_{|\partial B_1} = u_{*|\partial B_1}$. Such a function exists by classical results (see e.g. [126, Proposition 3.1]). Define $w_n \colon B_1 \to \mathbf{S}_0$ by

$$w_n(x) := \begin{cases} \varphi_n(x) & \text{if } x \in B_1 \setminus B_{1-\nu_n} \\ w_*\left(\dfrac{x}{1-\nu_n}\right) & \text{if } x \in B_{1-\nu_n}. \end{cases}$$

The function w_n is an admissible comparison function for u_n, i.e. $w_n \in H^1(B_1, \mathbf{S}_0)$ and $w_{n|\partial B_1} = u_{n|\partial B_1}$. Hence,

$$E_{\epsilon_n}(u_n, B_1) \leq E_{\epsilon_n}(w_n, B_1) = \frac{1-\nu_n}{2}\int_{B_1} |\nabla w_*|^2 + E_{\epsilon_n}(w_n, B_1 \setminus B_{1-\nu_n}).$$

When we take the limit as $n \to +\infty$, $\nu_n \to 0$ and the energy in the shell $B_1 \setminus B_{1-\nu_n}$ converges to 0, due to (2.4.14). Keeping (2.4.10) in mind, we obtain

$$\begin{aligned} \frac{1}{2}\int_{B_1} |\nabla u_*|^2 &\leq \liminf_{n\to+\infty} \frac{1}{2}\int_{B_1} |\nabla u_n|^2 \leq \limsup_{n\to+\infty} \frac{1}{2}\int_{B_1} |\nabla u_n|^2 \\ &\leq \limsup_{n\to+\infty} E_{\epsilon_n}(u_n, B_1) \leq \frac{1}{2}\int_{B_1} |\nabla w_*|^2 \leq \frac{1}{2}\int_{B_1} |\nabla u_*|^2, \end{aligned}$$

where the last inequality follows by the minimality of w_*, (2.4.15). But this implies

$$\lim_{n\to+\infty} \frac{1}{2}\int_{B_1} |\nabla u_n|^2 = \frac{1}{2}\int_{B_1} |\nabla u_*|^2,$$

which yields the strong H^1 convergence $u_n \to u_*$, as well as

$$\lim_{n\to+\infty} \frac{1}{\epsilon_n}\int_{B_1} f(u_n) = 0. \tag{2.4.16}$$

Moreover, u_* must be a minimizing harmonic map.

Scaling back to Q_{ε_n}, Q_0, we have shown that $Q_{\varepsilon_n} \to Q_0$ strongly in $H^1(B_r, \mathbf{S}_0)$ and that Q_0 is minimizing harmonic in B_r, where $r \geq \theta R$. In particular, the proposition holds true. □

Once Proposition 2.4.3 is established, Proposition 2.4.4 can be proved arguing as in Majumdar and Zarnescu's paper [98].

Remark 2.4.1. As a byproduct of the previous proof (see Equation (2.4.16)), we obtain the condition

$$\lim_{n\to+\infty} \frac{1}{\varepsilon_n^2} \int_{B_{\theta R}(x_0)} f(Q_{\varepsilon_n}) = 0,$$

which is essential for Majumdar and Zarnescu's analysis. Indeed, combining this information with the monotonicity formula (Lemma 2.2.12) and the $W^{1,\infty}$-estimate (Lemma 2.2.11), one deduces

$$\lim_{n\to+\infty} f(Q_{\varepsilon_n}) = 0 \qquad \text{uniformly on each } K \subset\subset B_{\theta R} \setminus \mathscr{S}_{\mathrm{pts}}$$

(see [98, Proposition 4]). Then, due to (F_2), one has $\mathrm{dist}(Q_{\varepsilon_n}(x), \mathscr{N}) \to 0$ locally uniformly in $B_{\theta R} \setminus \mathscr{S}_{\mathrm{pts}}$. This fact allows to obtain a Bochner inequality (see [98, Lemma 6]), and conclude via a Chen-Struwe type lemma (as in [32, Lemma 2.4]) that

$$\frac{1}{r} E_{\varepsilon_n}(Q_{\varepsilon_n}, B_r(x_0)) \leq C_1 \qquad \text{implies} \quad \sup_{x\in B_{r/2}(x_0)} r e_{\varepsilon_n}(Q_{\varepsilon_n}) \leq C_2$$

for some constants C_1, C_2 and any ball $B_r(x_0) \subseteq B_{\theta R} \setminus \mathscr{S}_{\mathrm{pts}}$ (see [98, Lemma 7]). Therefore, uniform convergence follows as in [98, Proposition 5].

2.4.3 The singular set

In this subsection, we complete the proof of Theorem 2.1.1 by defining the singular set $\mathscr{S}_{\mathrm{line}}$ and studying its properties. Throughout the subsection, we assume that Condition (H) holds. For each $0 < \varepsilon < 1$, define the measure μ_ε by

$$\mu_\varepsilon(B) := \frac{E_\varepsilon(Q_\varepsilon, B)}{|\log \varepsilon|} \qquad \text{for } B \in \mathscr{B}(\Omega). \tag{2.4.17}$$

In view of (H), the measures $\{\mu_\varepsilon\}_{0<\varepsilon<1}$ have uniformly bounded mass. Therefore, we may extract a subsequence $\varepsilon_n \searrow 0$ such that

$$\mu_{\varepsilon_n} \rightharpoonup^* \mu_0 \qquad \text{weakly}^\star \text{ in } \mathscr{M}_{\mathrm{b}}(\Omega) := C_0(\Omega)'. \tag{2.4.18}$$

Set $\mathscr{S}_{\mathrm{line}} := \mathrm{supp}\, \mu_0$. By definition, $\mathscr{S}_{\mathrm{line}}$ is a relatively closed subset of Ω.

Lemma 2.4.5. *For any $R_0 > 0$, there exists η with the following properties. Let $x_0 \in \Omega$, $0 < R < R_0$ be such that $B_R(x_0) \subseteq \Omega$. If*

$$\mu_0\left(\overline{B}_R(x_0)\right) < 2\eta R \tag{2.4.19}$$

then

$$\mu_0\left(B_{R/2}(x_0)\right) = 0,$$

that is $B_{R/2}(x_0) \subseteq \Omega \setminus \mathscr{S}_{\mathrm{line}}$.

Proof. In force of (2.4.18) and (2.4.19), we know that

$$\limsup_{n\to+\infty} \frac{E_{\varepsilon_n}(Q_{\varepsilon_n}, B_R(x_0))}{R \log(\varepsilon_n/R)} < 2\eta.$$

In particular, the assumption (2.1.10) is satisfied along the subsequence $\{\varepsilon_n\}$. Then, we can apply Proposition 2.1.6 with $\theta = 1/2$. From this and (2.4.19), we deduce

$$E_{\varepsilon_n}(B_{R/2}(x_0)) \leq MR$$

and hence, using (2.4.18),

$$\mu_0\left(B_{R/2}(x_0)\right) \leq \liminf_{n\to+\infty} \mu_{\varepsilon_n}\left(B_{R/2}(x_0)\right) = 0. \qquad \square$$

By the monotonicity formula (Lemma 2.2.12), for any $x \in \Omega$ the function

$$r \in (0, \operatorname{dist}(x, \partial\Omega)) \mapsto \frac{\mu_0\left(\overline{B}_r(x)\right)}{2r}$$

is non-decreasing, so the limit

$$\Theta(x) := \lim_{r \to 0^+} \frac{\mu_0\left(\overline{B}_r(x)\right)}{2r}$$

exists. The function Θ is usually called (1-dimensional) density of μ_0 (see [131, p. 10]).

Lemma 2.4.6. *For all $x \in \mathscr{S}_{\mathrm{line}}$, $\Theta(x) \geq \eta$.*

Proof. This follows immediately by Lemma 2.4.5. Indeed, if $x \in \mathscr{S}_{\mathrm{line}}$ then for any $r > 0$ we have $\mu_0(B_r(x)) > 0$, so Lemma 2.4.5 implies

$$\frac{\mu_0(\overline{B}_{2r}(x))}{4r} \geq \eta.$$

Passing to the limit as $r \to 0$, we conclude. ☐

Although elementary, this fact has remarkable consequences.

Proposition 2.4.7. *The set $\mathscr{S}_{\mathrm{line}}$ is countably $\mathscr{H}^1$-rectifiable, with $\mathscr{H}^1(\mathscr{S}_{\mathrm{line}}) < +\infty$. Moreover, the measure μ_0 can be written as $\mu_0 = \Theta\mathscr{H}^1 \llcorner \mathscr{S}_{\mathrm{line}}$, that is*

$$\mu_0(B) = \int_{B \cap \mathscr{S}_{\mathrm{line}}} \Theta(x)\, \mathrm{d}\mathscr{H}^1(x) \qquad \textit{for all } B \in \mathscr{B}(\Omega). \tag{2.4.20}$$

Proof. Lemma 2.4.6, together with [131, Theorem 3.2.(i), Chapter 1] and (H), implies

$$\mathscr{H}^1(\mathscr{S}_{\mathrm{line}}) \leq \eta^{-1}\mu_0(\Omega) \leq \eta^{-1} M < +\infty.$$

Moreover, since the 1-dimensional density of μ_0 exists and is positive μ_0-a.e., the support of μ_0 is a $\mathscr{H}^1$-rectifiable set and μ_0 is absolutely continuous with respect to $\mathscr{H}^1 \llcorner \mathscr{S}_{\mathrm{line}}$. This fact was proved by Moore [104] and is a special case of Preiss' theorem [115, Theorem 5.3], which holds true for measures in $\mathbb{R}^n$ having positive k-dimensional density, for any $k \leq n$. (For a self-contained presentation of Preiss' work, the reader is also referred to [39].) Thus, there exists a positive, $\mathscr{H}^1$-integrable function $g \colon \Omega \to \mathbb{R}$ such that

$$\mu_0(B) = \int_{B \cap \mathscr{S}_{\mathrm{line}}} g(x)\, \mathrm{d}\mathscr{H}^1(x) \qquad \text{for all } B \in \mathscr{B}(\Omega). \tag{2.4.21}$$

By Besicovitch differentiation theorem, there holds

$$\lim_{r \to 0^+} \frac{\mu_0(\overline{B}_r(x))}{\mathscr{H}^1(B_r(x) \cap \mathscr{S}_{\mathrm{line}})} = g(x) \qquad \text{for } \mathscr{H}^1\text{-a.e. } x \in \mathscr{S}_{\mathrm{line}}.$$

On the other hand, because $\mathscr{S}_{\mathrm{line}}$ is rectifiable and $\mathscr{H}^1(\mathscr{S}_{\mathrm{line}}) < +\infty$, [47, Theorem 3.2.19] implies that

$$\lim_{r \to 0^+} \frac{\mathscr{H}^1(B_r(x) \cap \mathscr{S}_{\mathrm{line}})}{2r} = 1 \qquad \text{for } \mathscr{H}^1\text{-a.e. } x \in \mathscr{S}_{\mathrm{line}}.$$

By combining these facts and (2.4.3), we obtain $\Theta = g$ $\mathscr{H}^1$-a.e. on $\mathscr{S}_{\mathrm{line}}$, so the proposition follows. ☐

The monotonicity of the energy, established in Lemma 2.2.12, provides a lower bound for the Hausdorff dimension of the singular set $\mathscr{S}_{\mathrm{line}}$.

Lemma 2.4.8. *For any open set $K \subset\subset \Omega$, either $\mathscr{S}_{\mathrm{line}} \cap K = \emptyset$ or the Hausdorff dimension of $\mathscr{S}_{\mathrm{line}} \cap K$ is* 1.

Proof. If $\mu_0(K) = 0$ then $K \cap \mathscr{S}_{\text{line}} =$ and the lemma is proved. Now, we assume that $\mu_0(K) > 0$. By Proposition 2.4.7 we know that $\mathscr{H}^1(\mathscr{S}_{\text{line}} \cap K) < +\infty$, so the dimension of $\mathscr{H}^1(\mathscr{S}_{\text{line}} \cap K)$ is at most 1. To check that it is exactly equal to 1, it suffices to show that $\mathscr{H}^1(\mathscr{S}_{\text{line}} \cap K) > 0$. Fix $0 < r_0 < \operatorname{dist}(K, \partial\Omega)$. By the monotonicity formula (Lemma 2.2.12) and the assumption (H), we have

$$\frac{E_\varepsilon(Q_\varepsilon, B_r(x))}{2r} \leq \frac{E_\varepsilon(Q_\varepsilon, B_{r_0}(x))}{2r_0} \leq \frac{M}{2r_0} |\log \varepsilon|$$

for any $0 < r < r_0$ and $x \in K$. Passing to the limit as $\varepsilon \to 0$, owning to (2.4.18) we have

$$\frac{\mu_0(\overline{B}_{r/2}(x))}{2r} \leq \frac{\mu_0(B_r(x))}{2r} \leq \frac{M}{2r_0}$$

and, in the limit as $r \to 0^+$, we obtain $\Theta(x) \leq M r_0^{-1}$ for any $x \in K$. Then, [131, Theorem 3.2.(2)] implies

$$\mathscr{H}^1(\mathscr{S}_{\text{line}} \cap K) \geq \frac{r_0}{2M} \mu_0(\mathscr{S}_{\text{line}} \cap K) > 0. \qquad \square$$

To complete the proof of Theorem 2.1.1, we check that Q_{ε_n} locally converge to a harmonic map, away from $\mathscr{S}_{\text{line}}$.

Proposition 2.4.9. *There exists a map $Q_0 \in H^1_{\text{loc}}(\Omega \setminus \mathscr{S}_{\text{line}}, \mathscr{N})$ such that, up to a relabeled subsequence,*

$$Q_{\varepsilon_n} \to Q_0 \qquad \textit{stongly in } H^1_{\text{loc}}(\Omega \setminus \mathscr{S}_{\text{line}}, \mathbf{S}_0).$$

The map Q_0 is minimizing harmonic on every ball $B \subset\subset \Omega \setminus \mathscr{S}_{\text{line}}$. Moreover, there exists a locally finite set $\mathscr{S}_{\text{pts}} \subseteq \Omega \setminus \mathscr{S}_{\text{line}}$ such that Q_0 is of class C^∞ on $\Omega \setminus (\mathscr{S}_{\text{line}} \cup \mathscr{S}_{\text{pts}})$, and

$$Q_{\varepsilon_n} \to Q_0 \qquad \textit{locally uniformly in } \Omega \setminus (\mathscr{S}_{\text{line}} \cup \mathscr{S}_{\text{pts}}).$$

Proof. Let $\{K^p\}_{p\in\mathbb{N}}$ be an increasing sequence of subsets $K^p \subset\subset \Omega \setminus \mathscr{S}_{\text{line}}$, such that $K^p \nearrow \Omega \setminus \mathscr{S}_{\text{line}}$. For each $p \in \mathbb{N}$, the compactness of K^p implies that there exists a finite covering of K^p with balls $\{B(x_i^p, r_i^p)\}_{1\leq i\leq I_p}$ such that

$$\overline{B}(x_i^p, 4r_i^p) \subseteq \Omega \setminus \mathscr{S}_{\text{line}} \qquad \text{i.e.} \qquad \mu_0\left(\overline{B}(x_i^p, 4r_i^p)\right) = 0. \tag{2.4.22}$$

Due to (2.4.18), this implies

$$\limsup_{n\to+\infty} \frac{E_{\varepsilon_n}(Q_{\varepsilon_n}, B(x_i^p, 4r_i^p))}{r_i^p \log(\varepsilon_n / r_i^p)} = 0$$

for each i, p. In particular, Condition (2.1.10) is satisfied. Applying Proposition 2.1.6 with $\theta = 1/2$, we infer

$$E_{\varepsilon_n}(Q_{\varepsilon_n}, B(x_i^p, 2r_i^p)) \leq C = C(i, p).$$

By Proposition 2.4.3 we deduce that, up to a relabeled subsequence, Q_{ε_n} converges strongly in H^1 to a map $Q_0 \in H^1(B(x_i^p, r_i^p), \mathscr{N})$. This is true for every $i \in \{1, \ldots, I_p\}$ so, after a further extraction of subsequences, we obtain

$$Q_{\varepsilon_n} \to Q_0 \quad \text{strongly in } H^1(K^p, \mathbf{S}_0), \quad \text{for all } p \in \mathbb{N}. \tag{2.4.23}$$

A priori, the subsequence $\{Q_{\varepsilon_n}\}$ depends on p, but one can use a diagonal argument to ensure that (2.4.23) is satisfied by *the same* subsequence, for all $p \in \mathbb{N}$.

For each ball $B \subset\subset \Omega \setminus \mathscr{S}_{\text{line}}$, the map Q_0 is minimizing harmonic on B. Indeed, fix a larger concentric ball B', with $B \subset\subset B' \subset\subset \Omega \setminus \mathscr{S}_{\text{line}}$. Denote by r, r' the radii of B, B' respectively. Because of $\mu_0(B') = 0$ and (2.4.18), one has

$$\limsup_{n\to+\infty} \frac{E_{\varepsilon_n}(Q_{\varepsilon_n}, B'}{r' \log(\varepsilon_n / r')} = 0.$$

As before, one applies Proposition 2.1.6, then Proposition 2.4.3, and obtains that Q_0 is minimizing harmonic on a ball of radius $\theta^2 r'$, for an arbitrarily fixed $0 < \theta < 1$. Taking θ so large that $\theta^2 r' > r$, it follows that Q_0 is minimizing harmonic on B.

Thanks to Schoen and Uhlenbeck's partial regularity result [125, Theorem II], we know that on each ball $B \subset\subset \Omega \setminus \mathscr{S}_{\mathrm{line}}$ there exists a finite set $X_B \subseteq B$ such that $Q_0 \in C^\infty(B \setminus X_B, \mathbf{S}_0)$. Therefore, $Q_0 \in C^\infty(\Omega \setminus \mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$, where $\mathscr{S}_{\mathrm{pts}} := \cup_B X_B$ is locally finite in $\Omega \cup \mathscr{S}_{\mathrm{line}}$. The locally uniform convergence $Q_{\varepsilon_n} \to Q_0$ on $\Omega \setminus (\mathscr{S}_{\mathrm{line}} \cup \mathscr{S}_{\mathrm{pts}})$ follows by Proposition 2.4.4, combined with a covering argument. ☐

We conclude our discussion about the properties of the singular set by proving that μ_0 is a stationary varifold. This will prove Proposition 2.1.2. These objects, introduced by Almgren [4], can be thought as weak counterparts of manifolds with vanishing mean curvature. For more details, the reader is referred to the paper by Allard [3] or the book by Simon [131]. (Actually, these authors use a slightly different terminology: what Simon calls a varifold corresponds to a rectifiable varifold in the sense of Almgren and Allard). Equation (2.4.20) implies that μ_0 is a rectifiable varifold; using the notation of [131, Chapter 4], we have $\mu_0 = \mu_{\mathbf{V}_0}$, where $\mathbf{V}_0 := \mathbf{V}(\mathscr{S}_{\mathrm{line}}, \Theta)$.

Before stating the following proposition, let us recall a basic fact. The rectifiability condition (2.4.21) for μ_0, together with [131, Remarks 1.9 and 11.5, Theorem 11.6], implies that for μ_0-a.e. x there exists a unique 1-dimensional subspace $L_x \subseteq \mathbb{R}^n$ such that

$$\lim_{\lambda \to 0} \int_{\mathbb{R}^d} \lambda^{-1} \phi\left(\frac{z-x}{\lambda}\right) \mathrm{d}\mu_0(z) = \Theta(x) \int_{L_x} \phi(y)\, \mathrm{d}\mathscr{H}^1(y) \qquad \text{for all } \phi \in C_c(\mathbb{R}^3). \tag{2.4.24}$$

Such line is called the *approximate tangent line* of μ_0 at x, and noted $\mathrm{Tan}(\mu_0, x)$.

Proposition 2.4.10. *The varifold $\mathbf{V}_0$ is stationary, i.e. for any vector field $X \in C^1_c(\Omega, \mathbb{R}^3)$ there holds*

$$\int_\Omega A_{ij}(x) \frac{\partial X^i}{\partial x_j}(x)\, \mathrm{d}\mu_0(x) = 0,$$

where the matrix $A(x) \in \mathrm{M}_3(\mathbb{R})$ represents the orthogonal projection on $\mathrm{Tan}(\mu_0, x)$, for all $x \in \Omega$.

Proof. The proposition follows by adapting Ambrosio and Soner's analysis in [6]. For the convenience of the reader, we give here the proof. Define the matrix-valued map $A^\varepsilon = (A^\varepsilon_{ij})_{i,j} \colon \Omega \to \mathrm{M}_3(\mathbb{R})$ by

$$A^\varepsilon_{ij} := \frac{1}{|\log \varepsilon|}\left(e_\varepsilon(Q_\varepsilon)\delta_{ij} - \frac{\partial Q_\varepsilon}{\partial x_i} \cdot \frac{\partial Q_\varepsilon}{\partial x_j}\right) \qquad \text{for } i, j \in \{1,\, 2,\, 3\}.$$

Then A^ε is a symmetric matrix, such that

$$\operatorname{tr} A^\varepsilon = \frac{1}{|\log \varepsilon|}\left(3 e_\varepsilon(Q_\varepsilon) - |\nabla Q_\varepsilon|^2\right) \geq \mu_\varepsilon \tag{2.4.25}$$

and

$$|A^\varepsilon| \leq C\mu_\varepsilon. \tag{2.4.26}$$

For any vector $v \in \mathbb{S}^2$, there holds

$$A^\varepsilon_{ij} v_i v_j = \frac{1}{|\log \varepsilon|}\left(e_\varepsilon(Q_\varepsilon) - \left|v_i \frac{\partial Q_\varepsilon}{\partial x_i}\right|^2\right) \leq \mu_\varepsilon, \tag{2.4.27}$$

so the eigenvalues of A^ε are less or equal than μ_ε. Moreover, integrating by parts the stress-energy identity (Lemma 2.2.13) we obtain

$$\int_\Omega A^\varepsilon_{ij}(x) \frac{\partial X^i}{\partial x_j}(x)\, \mathrm{d}x = 0 \qquad \text{for any } X \in C^1_c(\Omega, \mathbb{R}^3). \tag{2.4.28}$$

In view of (2.4.26), and extracting a subsequence if necessary, we have that $A^\varepsilon \rightharpoonup^* A^0$ in the weak-$*$ topology of $\mathscr{M}(\Omega,\, \mathrm{M}_3(\mathbb{R})) = C_c(\Omega,\, \mathrm{M}_3(\mathbb{R}))'$. The limit measure A^0 satisfies $|A^0| \leq C\mu_0$, in particular is absolutely continuous with respect to μ_0. Therefore, there exists a matrix-valued function $A \in L^1(\Omega,\, \mu_0;\, \mathrm{M}_3(\mathbb{R}))$ such that

$$\mathrm{d}A^0(x) = A(x)\mathrm{d}\mu_0(x) \qquad \text{as measures in } \mathscr{M}(\Omega,\, \mathrm{M}_3(\mathbb{R})).$$

Passing to the limit in (2.4.25), (2.4.27) and (2.4.28), for μ_0-a.e. x we obtain that $A(x)$ is a symmetric matrix, with $\operatorname{tr} A(x) \geq 1$ and eigenvalues less or equal than 1, such that

$$\int_\Omega A_{ij}(x)\frac{\partial X^i}{\partial x_j}(x)\mathrm{d}\mu_0(x) = 0 \qquad \text{for any } X \in C^1_c(\Omega,\, \mathbb{R}^3). \tag{2.4.29}$$

Now, fix a Lebesgue point x for A (with respect to μ_0) and $0 < \lambda < \mathrm{dist}(x,\, \partial\Omega)$. Condition (2.4.29) implies

$$\lambda^{-1}\int_{\mathbb{R}^3} A(z)\cdot \nabla X\left(\frac{z-x}{\lambda}\right)\mathrm{d}\mu_0(z) = 0 \qquad \text{for any } X \in C^1_c(B_1,\, \mathbb{R}^3). \tag{2.4.30}$$

Then,

$$\begin{aligned}&\left|\lambda^{-1}\int_{\mathbb{R}^3}(A(z) - A(x))\cdot\nabla X\left(\frac{z-x}{\lambda}\right)\mathrm{d}\mu_0(x)\right| \\ &\qquad\qquad \leq \underbrace{\frac{\mu_0(\overline{B}_\lambda(x))}{\lambda}}_{\to\Theta(x)/2}\|\nabla X\|_{L^\infty(B_1)}⨍_{B_\lambda(x)}|A(z) - A(x)|\, d\mu_0(z) \to 0\end{aligned}$$

as $\lambda \to 0$. Combined with (2.4.24) and (2.4.30), this provides

$$\Theta(x)A(x)\cdot\int_{\mathrm{Tan}(\mu_0,x)}\nabla X\,\mathrm{d}\mathscr{H}^1 = \lim_{\lambda\to 0}\lambda^{-1}\int_{\mathbb{R}^3}A(x)\cdot\nabla X\left(\frac{z-x}{\lambda}\right)\mathrm{d}\mu_0(x) = 0$$

for any $X \in C^1_c(B_1,\, \mathbb{R}^3)$. Since $\Theta(x) > 0$ by Lemma 2.4.6, applying [6, Lemma 3.9] (with $\beta = s = 1$ and $\nu = \frac{1}{2}\mathscr{H}^1 \llcorner \mathrm{Tan}(\mu_0, x)$) we deduce that at least two eigenvalues of $A(x)$ vanish, for μ_0-a.e. x. On the other hand, we know already that $\operatorname{tr} A(x) = 1$ with eigenvalues ≤ 1. Therefore, the eigenvalues of $A(x)$ are $(1,\, 0,\, 0)$ and $A(x)$ represents the orthogonal projection on a line.

Let $\mathbf{G}_{1,3} \subseteq \mathrm{M}_3(\mathbb{R})$ be the set of matrices representing orthogonal projections on 1-subspaces of $\mathbb{R}^3$. The push-forward measure $\mathbf{V} := (\mathrm{Id},\, A)_{\#}\mu_0$, i.e. the measure $\mathbf{V} \in \mathscr{M}(\Omega \times \mathbf{G}_{1,3})$ given by

$$\int_{\Omega\times\mathbf{G}_{1,3}}\varphi(x,\, M)\,\mathrm{d}\mathbf{V}(x,\, M) := \int_\Omega \varphi(x,\, A(x))\,\mathrm{d}\mu_0(x) \qquad \text{for } \varphi \in C_c(\Omega\times\mathbf{G}_{1,3}), \tag{2.4.31}$$

is a varifold (in the sense of Almgren), and condition (2.4.29) means precisely that $\mathbf{V}$ is stationary. A classical result by Allard (see [3] or [6, Theorem 3.3]) asserts that every varifold with locally bounded first variation and positive density is rectifiable. In our case, $\mathbf{V}$ has vanishing first variation, and the density is bounded from below by Lemma 2.4.6. Therefore, by Allard's theorem $\mathbf{V}$ is rectifiable. In particular $A(x)$ is the orthogonal projection on $\mathrm{Tan}(\mathscr{S}_{\mathrm{line}},\, x)$, for μ_0-a.e. x. □

2.5 Sufficient conditions for (H). The role of the boundary data

2.5.1 Proof of Propositions 2.1.4 and 2.1.5

In this section, we analyze the role of the domain and the boundary data in connection with (H), and prove sufficient conditions for (H) to hold true. We prove first Proposition 2.1.4, namely, we show that an assumption on the topology of Ω combined with a logarithmic upper bound on the energy of the boundary data (see (H_2)–(H_3)) imply

$$\|Q_\varepsilon\|_{L^\infty(\Omega)} \leq M \tag{2.5.1}$$

and

$$E_\varepsilon(Q_\varepsilon) \leq M\left(|\log\varepsilon| + 1\right), \tag{2.5.2}$$

for some positive constant $M = M(\Omega,\, M_0)$. At the end of the subsection, we also prove Proposition 2.1.5.

Lemma 2.5.1. *Minimizers* Q_ε *of* $(\mathrm{LG}_\varepsilon)$ *satisfy*

$$\|Q_\varepsilon\|_{L^\infty(\Omega)} \leq \max\left\{\sqrt{\frac{2}{3}}s_*,\ \|g_\varepsilon\|_{L^\infty(\partial\Omega)}\right\}.$$

Proof. Set

$$M := \max\left\{\sqrt{\frac{2}{3}}s_*,\ \|Q_\varepsilon\|_{L^\infty(\partial\Omega)}\right\},$$

and define $\varrho\colon \mathbf{S}_0 \to \mathbf{S}_0$ by $\varrho(Q) := M|Q|^{-1}Q$ if $|Q| \geq M$, $\varrho(Q) := Q$ otherwise. We have

$$\mathrm{D}f(Q)\cdot Q = -a\,|Q|^2 - b\operatorname{tr}Q^3 + c\,|Q|^4 > 0 \qquad \text{when } |Q| > \sqrt{\frac{2}{3}}s_*$$

(this follows from the inequality $\sqrt{6}|\operatorname{tr}Q^3| \leq |Q|^3$; see [95]). We deduce that $f(\varrho(Q)) \geq f(Q)$ for any Q. Moreover, ϱ is the projection on a convex set, so it is 1-Lipschitz continuous. Thus, the map $P_\varepsilon := \varrho(Q_\varepsilon)$ belongs to $H^1_{g_\varepsilon}(\Omega,\, \mathbf{S}_0)$, satisfies $|\nabla P_\varepsilon| \leq |\nabla Q_\varepsilon|$ a.e. and $E_\varepsilon(P_\varepsilon) \leq E_\varepsilon(Q_\varepsilon)$, with strict inequality if $|Q_\varepsilon| > M$ on a set of positive measure. This would contradict the minimality of Q_ε, so $|Q_\varepsilon| \leq M$ a.e. $\square$

Now, we prove the energy bound (2.5.2) by constructing an admissible comparison function whose energy is controlled by the right-hand side of (2.5.2). If Ω is a ball, it sufficies to extend homogeneously the boundary data, thanks to (H_3). Since Ω is bilipschitz equivalent to a handlebody by (H_2), we can reduce to the case of a ball by cutting each handle of Ω along a meridian disk. This technique was used already in [60, Lemma 1.1]. The following lemma allow us to extend the boundary datum to the interior of the cut disks. Unlike the results of Section 2.3, in this lemma we do not constrain the extension to take values in $\mathscr{N}$. Instead, we prescribe a logarithmic upper bound for its energy.

Lemma 2.5.2. *There exists a constant* $C > 0$ *such that, for any* $0 < \varepsilon < 1$ *and any function* $g \in H^1(\partial B^2_1,\, \mathscr{N})$*, there exists* $v \in H^1(B^2_1,\, \mathbf{S}_0)$ *such that* $v_{\varepsilon|\partial B^2_1} = g$ *and*

$$E_\varepsilon(v,\, B^2_1) \leq C\left(\int_{\partial B^2_1} |\nabla g|^2 \,\mathrm{d}\mathscr{H}^1 + |\log\varepsilon| + 1\right).$$

Proof. In view of the Sobolev embedding $H^1(\partial B^2_1, \mathbf{S}_0) \hookrightarrow C^0(\partial B^2_1,\, \mathbf{S}_0)$, it makes sense to consider the homotopy class of g. If g is homotopically trivial, it may be extended to a function in $H^1(B^2_1,\, \mathbf{S}_0)$, still denoted g by simplicity. Then, Lemma 2.3.2 provides a function v with the desired properties.

Assume now that g is not homotopically trivial, and fix arbitrarily another homotopically trivial loop $h \in H^1(\partial B^2_{1/2},\, \mathscr{N})$. For instance, choose $h(x) = P(2x)$ for $x \in \partial B^2_{1/2}$, where P is given by Lemma 2.2.9. It is easy to check that the function

$$w_\varepsilon(x) := \eta_\varepsilon(|x|)h\left(\frac{x}{|x|}\right) \qquad \text{for } x \in B^2_{1/2},$$

where

$$\eta_\varepsilon(r) := \begin{cases} 1 & \text{if } r \geq \varepsilon \\ \varepsilon^{-1} r & \text{if } 0 \leq r < \varepsilon, \end{cases} \tag{2.5.3}$$

belongs to $H^1(B^2_{1/2}, \mathbf{S}_0)$ and

$$E_\varepsilon(w_\varepsilon, B^2_{1/2}) \leq C\, |\log \varepsilon| \int_{\partial B^2_{1/2}} |\nabla_\top h|^2 \, \mathrm{d}\mathscr{H}^1 + C \leq C\, (|\log\varepsilon| + 1)\,. \tag{2.5.4}$$

Indeed,

$$|\nabla w_\varepsilon|^2 = \left|\frac{\mathrm{d}w_\varepsilon}{\mathrm{d}r}\right|^2 + \frac{1}{r^2}\, |\nabla_\top w_\varepsilon|^2 \begin{cases} \leq C\varepsilon^{-1} & \text{where } r \leq \varepsilon \\ = r^{-2}|\nabla_\top h|^2 & \text{where } r \geq \varepsilon, \end{cases}$$

and $w_\varepsilon(x) \in \mathscr{N}$ if $|x| \geq \varepsilon$. Therefore, we have

$$\begin{aligned} E_\varepsilon(w_\varepsilon, B^2_{1/2}) &\leq \int_\varepsilon^{1/2} \frac{\mathrm{d}r}{r} \int_{\mathbb{S}^1} |\nabla_\top h|^2 \, \mathrm{d}\mathscr{H}^1 + E_\varepsilon(w_\varepsilon, B^2_\varepsilon) \\ &\leq (|\log \varepsilon| - \log 2) \int_{\mathbb{S}^1} |\nabla_\top h|^2 \, \mathrm{d}\mathscr{H}^1 + C, \end{aligned}$$

whence (2.5.4) follows.

To complete the proof of the lemma, we only need to interpolate between g and h by a function defined on the annulus $D := B^2_1 \setminus B^2_{1/2}$. Up to a bilipschitz equivalence, D can be thought as the unit square $(0, 1)^2$ with an equivalence relation identifying two opposite sides of the boundary, as shown in Figure 2.3. We assign the boundary datum g on the bottom side, and h on the top side. Since $\mathscr{N}$ is path-connected, we find a smooth path $c\colon [0, 1] \to \mathscr{N}$ connecting $g(0, 0)$ to $h(0, 1)$. By assigning c as a boundary datum on the lateral sides of the square, we have defined an H^1-map $\partial[0, 1]^2 \to \mathscr{N}$, homotopic to $g{*}c{*}h{*}\tilde{c}$. (Here, the symbol $*$ stands for composition of paths, and $\tilde{c}$ is the reverse path of c). Since the square is bilipschitz equivalent to a disk, it is possible to apply Lemma 2.3.2 and find $\tilde{v} \in H^1([0, 1]^2, \mathscr{N})$ such that

$$\int_{[0,1]^2} |\nabla \tilde{v}|^2 \, \mathrm{d}\mathscr{H}^2 \leq C \left(\|\nabla g\|^2_{L^2(\partial B^2_1)} + \|\nabla h\|^2_{L^2(\partial B^2_{1/2})} + \|c'\|^2_{L^2(0,1)} \right). \tag{2.5.5}$$

Passing to the quotient $[0, 1]^2 \to D$, we obtain a map $v \in H^1(D, \mathbf{S}_0)$. We extend v by setting $v := w_\varepsilon$ on $B^2_{1/2}$. The lemma now follows from (2.5.4) and (2.5.5), because the H^1-norms of both h and c are controlled by a constant depending only on $\mathscr{N}$. ☐

In the following lemma, we construct cut disks with suitable properties.

Lemma 2.5.3. *Assume that* (H$_2$) *and* (H$_3$) *hold. There exists a finite number of properly embedded disks*[3] $D_1, D_2, \ldots, D_k \subseteq \Omega$ *such that* $\Omega \setminus \cup_{i=1}^k D_i$ *is diffeomorphic to a ball,*

$$E_\varepsilon(g_\varepsilon, \partial D_i) \leq C\, (|\log\varepsilon| + 1) \tag{2.5.6}$$

and

$$\mathrm{dist}(g_\varepsilon(x), \mathscr{N}) \to 0 \qquad \textit{uniformly in } x \in \bigcup_{i=1}^k \partial D_i. \tag{2.5.7}$$

3. By saying that D_i is *properly* embedded, we mean that $\partial D_i = D_i \cap \partial\Omega$ and D_i is transverse to $\partial\Omega$ at each point of ∂D_i.

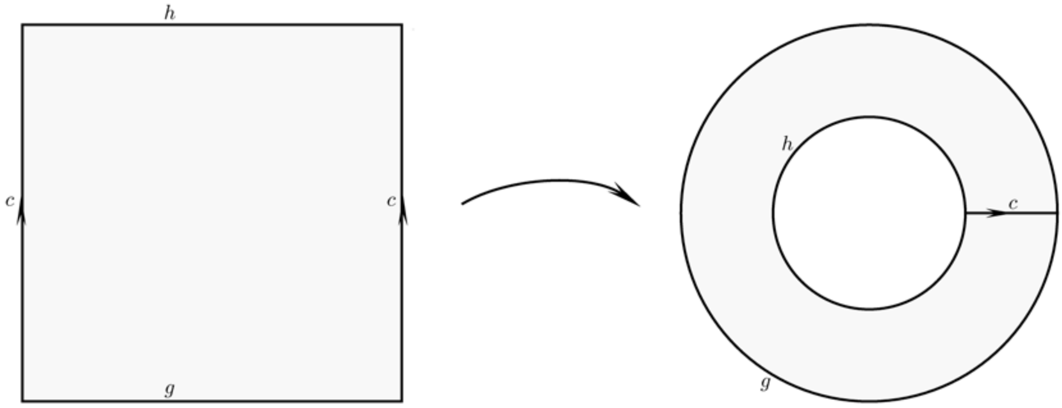


Figure 2.3: A square can be mapped into an annulus, by identifying a pair of opposite sides.

Proof. For each handle i of Ω, there is an open set U_i such that $\partial\Omega \cap U_i$ is foliated by

$$\partial\Omega \cap U_i = \coprod_{-a_0<a<a_0} \partial D_i^a,$$

where the generic D_i^a is a properly embedded disk, which cross transversely a generator of $\pi_1(\Omega)$ at some point. Then, Fatou's lemma implies that

$$\int_{-a_0}^{a_0} \liminf_{\varepsilon\to 0} E_\varepsilon(g_\varepsilon,\, \partial D_i^a)\,\mathrm{d}a \leq \liminf_{\varepsilon\to 0} \int_{-a_0}^{a_0} E_\varepsilon(g_\varepsilon,\, \partial D_i^a)\,\mathrm{d}a \overset{(\mathrm{H}_3)}{\leq} C\left(|\log\varepsilon| + 1\right),$$

so, by an average argument, we can choose the parameter a in such a way that $D_i := D_i^a$ satisfies (2.5.6). Then, (2.5.7) is obtained by the same arguments as Lemma 2.3.11. (As in the lemma, we apply Sobolev-Morrey's embedding inequality not on ∂D_i directly, but on 1-cells $K \subseteq \partial D_i$ of size comparable to $\varepsilon^\alpha |\log\varepsilon|$). Furthermore, by construction $\Omega \setminus \cup_{i=1}^k D_i$ is a ball, since we have removed a meridian disk for each handle of Ω. □

Proof of Proposition 2.1.4. The L^∞-bound (2.5.1) holds by virtue of Lemma 2.5.1, so we only need to prove (2.5.2). Assume for a moment that $\Omega = B_1$. In this case, define the function

$$P_\varepsilon(x) := \eta_\varepsilon(|x|)g_\varepsilon\left(\frac{x}{|x|}\right) \qquad \text{for } x \in B_1, \tag{2.5.8}$$

where η_ε is given by (2.5.3). Then $P_\varepsilon \in H^1_{g_\varepsilon}(B_1,\, \mathbf{S}_0)$ and we easily compute

$$\begin{aligned}
E_\varepsilon(P_\varepsilon) &= E_\varepsilon(P_\varepsilon,\, B_1 \setminus B_\varepsilon) + E_\varepsilon(P_\varepsilon,\, B_\varepsilon) \\
&= \int_\varepsilon^1 \int_{\partial B_1} \left(|\nabla_\top g_\varepsilon|^2 + \varepsilon^{-2} r^2 f(g_\varepsilon)\right) \mathrm{d}\mathscr{H}^2\,\mathrm{d}r \\
&\qquad + \int_0^\varepsilon \int_{\partial B_1} \varepsilon^{-2} r^2 \left(|g_\varepsilon|^2 + |\nabla_\top g_\varepsilon|^2 + f(P_\varepsilon)\right) \mathrm{d}\mathscr{H}^2\,\mathrm{d}r.
\end{aligned}$$

In view of Assumption (H$_3$), this yields

$$E_\varepsilon(P_\varepsilon) \leq C\left(E_\varepsilon(g_\varepsilon,\, \partial B_1) + 1\right) \leq C\left(|\log\varepsilon| + 1\right),$$

so the lemma holds true when $\Omega = B_1$.

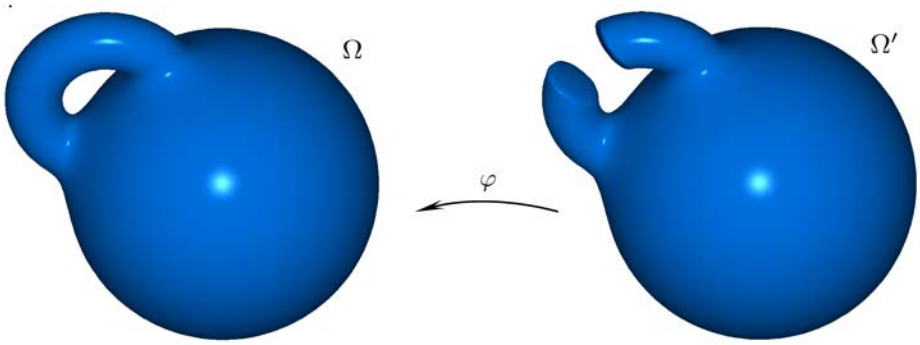


Figure 2.4: On the left, a ball with one handle. On the right, the corresponding domain Ω': the handle has been cut along a disk. The map $\varphi\colon \Omega' \to \Omega$ identifies the opposite disks in the handle cut.

Now, arguing as in [60, Lemma 1.1], we prove that the general case can be reduced to the previous one. Let Ω be any domain satisfying (H_2), and let $D_1, \ldots, D_k$ be the disks given by Lemma 2.5.3. By (2.5.7), there exists $\varepsilon_0 > 0$ such that, for any $0 < \varepsilon < \varepsilon_0$ and any $x \in \cup_i \partial D_i$,

$$\mathrm{dist}(g_\varepsilon(x), \mathscr{N}) \leq \delta_0.$$

For ease of notation, for a fixed $i \in \{1, \ldots, k\}$ we assume, up to a bilipschitz equivalence, that $D_i = B_1^2$. Then, we define $\hat{g}_{\varepsilon,i}\colon B_1^2 \to \mathbf{S}_0$ by

$$\hat{g}_{\varepsilon,i}(x) := \begin{cases} \dfrac{\delta_0 + |x| - 1}{\delta_0} g_\varepsilon\left(\dfrac{x}{|x|}\right) + \dfrac{1-|x|}{\delta_0}(\mathscr{R}\circ g_\varepsilon)\left(\dfrac{x}{|x|}\right) & \text{if } 1-\delta_0 \leq |x| \leq 1 \\ v_\varepsilon\left(\dfrac{x}{1-\delta_0}\right) & \text{if } |x| \leq 1-\delta_0, \end{cases}$$

where $v_\varepsilon \in H^1(B_1^2, \mathbf{S}_0)$ is the extension of $\mathscr{R}\circ g_{\varepsilon|\partial B_1^2}$ given by Lemma 2.5.2. By a straightforward computation, one checks that

$$E_\varepsilon(\hat{g}_{\varepsilon,i}, D_i) \leq C\left(E_\varepsilon(g_\varepsilon, \partial D_i) + |\log\varepsilon| + 1\right). \tag{2.5.9}$$

Now, consider two copies D_i^+ and D_i^- of each disk D_i. Let Ω' be a smooth domain such that

$$\Omega' \simeq (\Omega \setminus \cup_i D_i) \cup_i D_i^+ \cup_i D_i^-,$$

and let $\phi\colon \Omega' \to \Omega$ be the smooth map which identifies each D_i^+ with the corresponding D_i^- (see Figure 2.4). This new domain is simply connected, and in fact is diffeomorphic to a ball. Up to a bilipschitz equivalence, we will assume that Ω' *is* a ball. We define a boundary datum g'_ε for Ω' by setting $g'_\varepsilon := g_\varepsilon$ on $\Omega \setminus \cup_i D_i$, and $g'_\varepsilon := g_{\varepsilon,\,i}$ on $D_i^+ \cup D_i^-$. Then, (2.5.9), (2.5.6) and (H_3) imply

$$E_\varepsilon(g'_\varepsilon, \partial\Omega) \leq C\left(E_\varepsilon(g_\varepsilon, \partial\Omega) + |\log\varepsilon| + 1\right) \leq C\left(|\log\varepsilon| + 1\right).$$

Then Formula (2.5.8) gives a map $P'_\varepsilon \in H^1_{g'_\varepsilon}(\Omega', \mathbf{S}_0)$ which satisfies

$$E_\varepsilon(P'_\varepsilon, \Omega') \leq C\left(|\log\varepsilon| + 1\right).$$

Since $P'_{\varepsilon|D_i^+} = P'_{\varepsilon|D_i^-}$ for every i, the map P'_ε factorizes through ϕ, and defines a new function $P_\varepsilon \in H^1_{g_\varepsilon}(\Omega, \mathbf{S}_0)$ such that

$$E_\varepsilon(Q_\varepsilon, \Omega) \leq E_\varepsilon(P_\varepsilon, \Omega) \leq C\left(|\log\varepsilon| + 1\right). \qquad \square$$

We turn now to the proof of Proposition 2.1.5. The boundary data we construct are smooth approximations of a map $\partial\Omega \to \mathscr{N}$ with at least one point singularity. Then, the lower bound for the energy follows by the estimates of Subsection 2.2.2.

Proof of Proposition 2.1.5. Up to rotations and translations, we can assume that the x_3-axis $\{x_1 = x_2 = 0\}$ crosses transversely $\partial\Omega$ at one point x_0 at least. Let $\eta_\varepsilon \in C^\infty(\mathbb{R}^+, \mathbb{R})$ be a cut-off function satisfying

$$\eta_\varepsilon(0) = \eta_\varepsilon'(0) = 0, \qquad \eta_\varepsilon(r) = s_* \text{ for } r \geq \varepsilon, \qquad 0 \leq \eta_\varepsilon \leq s_*, \qquad |\eta_\varepsilon'| \leq C\varepsilon^{-1}.$$

Set

$$g_\varepsilon(x) := \eta_\varepsilon(|x'|) \left\{ \left(\frac{x'}{|x'|} \right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right\} \qquad \text{for } x \in \partial\Omega,$$

where $x' := (x_1, x_2, 0)$. Then, a straightforward computation shows that g_ε is of class C^1 and satisfies (H_3). The minimizers $Q_\varepsilon \in H^1_{g_\varepsilon}(\Omega, \mathbf{S}_0)$ of (LG_ε) are C^1-solutions of (2.2.23), by Lemma 2.5.1. The interpolation results of [13, Lemma A.1, A.2] imply

$$\|Q_\varepsilon\|_{L^\infty(\Omega)} + \varepsilon \|\nabla Q_\varepsilon\|_{L^\infty(\Omega)} \leq C. \tag{2.5.10}$$

Now, consider a ball $B_r(x_0)$. If the radius r is small enough, the set $\Omega \cap B_r(x_0)$ can be mapped diffeomorphically onto the half-ball

$$U := \left\{ x \in \mathbb{R}^3 \colon |x| \leq 1, \ x_3 \geq 0 \right\},$$

so we can assume without loss of generality that $\Omega \cap B_r(x_0) = U$. Let $U_s := \{x \in U \colon x_3 = s\}$, for $r/2 \leq s \leq r$. The map $Q_{\varepsilon|\partial U_s} \colon \partial U_s \to \mathscr{N}$ is a homotopically non-trivial loop, with

$$\|Q_\varepsilon\|_{W^{1,\infty}(\partial U_s)} \leq C = C(r, \Omega),$$

and Q_ε satisfies (2.5.10). Then, Corollary 2.2.6 applies, and we deduce

$$E_\varepsilon(Q_\varepsilon, U_s) \geq \kappa_* \log \frac{s}{\varepsilon} - C$$

for a constant C depending on r, Ω. By integrating this bound for $s \in (r/2, r)$, the proposition follows. □

Remark 2.5.1. Let $\{Q_\varepsilon\}$ be a sequence of minimizers and α be a positive number such that

$$E_\varepsilon(Q_\varepsilon) \geq \alpha \left(|\log \varepsilon| - 1 \right) \tag{2.5.11}$$

for any ε, as in Proposition 2.1.5. Let μ_ε be the measure defined by (2.4.17). Then, there exist a subsequence $\varepsilon_n \searrow 0$ and a bounded measure $\mu_0 \in \mathscr{M}_\mathrm{b}(\mathbb{R}^3)$ such that

$$\mu_{\varepsilon_n} \rightharpoonup^* \mu_0 \qquad \text{in } \mathscr{M}_\mathrm{b}(\mathbb{R}^3)$$

and $\mu_0(\overline{\Omega}) \geq \alpha > 0$. In particular, the support $\mathscr{S}_\mathrm{line}$ of μ_0 is a non-empty, closed subset of $\overline{\Omega}$. However, it might happen that $\mathscr{S}_\mathrm{line}$ is contained in the boundary of Ω, even if the boundary datum is regular. For instance, let the domain Ω be a solid torus, parametrized by the map

$$\phi \colon (\rho, \theta, \varphi) \in [0, 1) \times [0, 2\pi]^2 \mapsto \begin{cases} x_1 = (2 + \rho\cos\varphi)\cos\theta \\ x_2 = (2 + \rho\cos\varphi)\sin\theta \\ x_3 = \rho\sin\varphi. \end{cases}$$

Take the boundary datum $g_\varepsilon = g \in C^1(\partial\Omega, \mathscr{N})$ given by

$$g(\phi(1, \theta, \varphi)) = s_* \left\{ \left(\mathbf{e}_\theta \cos\frac{\varphi}{2} + \mathbf{e}_\varphi \sin\frac{\varphi}{2} \right)^{\otimes 2} - \frac{1}{3}\,\mathrm{Id} \right\},$$

where $\mathbf{e}_\theta := \partial_\theta\phi/|\partial_\theta\phi|$, $\mathbf{e}_\varphi := \partial_\varphi\phi$ are orthogonal tangent vectors on the torus. The restriction of g to each slice $\phi(\{1\} \times \{\theta\} \times [0, 2\pi])$ is homotopically non-trivial, so (2.5.11) is satisfied and $\mathscr{S}_\mathrm{line}$ is non-empty. Because of the minimality of Q_ε, we expect $\mathscr{S}_\mathrm{line}$ to be length-minimizing among the loops C such that $\phi([0, 1] \times \{\theta\} \times [0, 2\pi]) \cap C \neq \emptyset$ for all θ. Thus, we *conjecture* that

$$\mathscr{S}_\mathrm{line} = \left\{ x \in \mathbb{R}^3 \colon x_3 = 0, \ x_1^2 + x_2^2 = 1 \right\} \subseteq \partial\Omega.$$

In contrast, for the boundary data constructed in proof of Proposition 2.1.5 we expect that $\mathscr{S}_\mathrm{line}$ lies inside the domain (more precisely $\mathscr{S}_\mathrm{line} = \Omega \cap \{x_1 = x_2 = 0\}$), because of minimality arguments.

2.5.2 Proof of Proposition 2.1.3

If Ω is a bounded, Lipschitz domain and the boundary data are a bounded sequence in $H^{1/2}(\partial\Omega, \mathscr{N})$, then the logarithmic bound for minimizers holds as well. We will give now the proof of this fact, by adapting an argument by Rivière (see [118, Proposition 2.1]). Hardt, Kinderlehrer and Lin's re-projection trick (see Subsection 2.3.1) is a key point here.

Proof of Proposition 2.1.3. Once again, Lemma 2.5.1 directly gives the L^∞-bound (2.5.1), so we only need to prove (2.5.2) by constructing a suitable comparison function. For any $0 < \varepsilon < 1$, let $u_\varepsilon \in H^1(\Omega, \mathbf{S}_0)$ be the harmonic extension of g_ε, i.e. the unique solution of

$$\begin{cases} -\Delta u_\varepsilon = 0 & \text{in } \Omega \\ u_\varepsilon = g_\varepsilon & \text{on } \partial\Omega. \end{cases}$$

Then, since $(g_\varepsilon)_\varepsilon$ is bounded in $H^{1/2} \cap L^\infty$, the sequence $\{u_\varepsilon\}_\varepsilon$ is bounded in $H^1 \cap L^\infty$. Let $\delta > 0$ be a parameter to be chosen later. For any $A \in \mathbf{S}_0$ with $|A| \leq \delta$ and any ε, we define

$$u_\varepsilon^A := (\eta_\varepsilon \circ \phi)\,(u_\varepsilon - A)\,\mathscr{R}\,(u_\varepsilon - A)$$

where $\phi\colon \mathbf{S}_0 \to \mathbb{R}$ and $\mathscr{R}\colon \mathbf{S}_0 \backslash \mathscr{C} \to \mathscr{N}$ are defined respectively in Lemmas 2.2.3, 2.2.2, and $\eta_\varepsilon \in C(\mathbb{R}^+, \mathbb{R})$ is given by

$$\eta_\varepsilon(r) := \varepsilon^{-1} r \quad \text{if } 0 \leq r < \varepsilon, \qquad \eta_\varepsilon(r) = 1 \quad \text{if } r \geq \varepsilon.$$

By Lemma 2.2.2 and Corollary 2.2.8, we have $u_\varepsilon^A \in (H^1 \cap L^\infty)(\Omega, \mathbf{S}_0)$. We differentiate u_ε^A and, taking advantage of the Lipschitz continuity of ϕ (Lemma 2.2.3), we deduce

$$\left|\nabla u_\varepsilon^A\right|^2 \leq C \left\{ \left(\eta'_\varepsilon \circ \phi\right)^2 (u_\varepsilon - A) \left|\nabla u_\varepsilon\right|^2 + \left(\eta_\varepsilon \circ \phi\right)^2 (u_\varepsilon - A) \left|\nabla \left(\mathscr{R}(u_\varepsilon - A)\right)\right|^2 \right\}.$$

We apply Corollary 2.2.8 to bound the derivative of $\mathscr{R} \circ (u_\varepsilon - A)$:

$$\left|\nabla u_\varepsilon^A\right|^2 \leq C \left\{ \left(\eta'_\varepsilon \circ \phi\right)^2 (u_\varepsilon - A) + \frac{\left(\eta_\varepsilon \circ \phi\right)^2 (u_\varepsilon - A)}{\phi^2(u_\varepsilon - A)} \right\} \left|\nabla u_\varepsilon\right|^2.$$

On the other hand, there holds

$$f\left(u_\varepsilon^A\right) \leq C \mathbb{1}_{\{\phi(u_\varepsilon - A) \leq \varepsilon\}},$$

so

$$E_\varepsilon\left(u_\varepsilon^A\right) \leq C \int_\Omega \left\{ \left(\frac{\mathbb{1}_{\{\phi(u_\varepsilon - A) \geq \varepsilon\}}}{\phi^2(u_\varepsilon - A)} + \varepsilon^{-2} \mathbb{1}_{\{\phi(u_\varepsilon - A) \leq \varepsilon\}} \right) \left|\nabla u_\varepsilon\right|^2 + \varepsilon^{-2} \mathbb{1}_{\{\phi(u_\varepsilon - A) \leq \varepsilon\}} \right\}. \tag{2.5.12}$$

Now, fix a bounded subset $K \subseteq \mathbf{S}_0$, so large that $u_\varepsilon(x) + B_\delta^{\mathbf{S}_0} \subseteq K$ for a.e. $x \in \Omega$ and any ε (we denote by $B_\delta^{\mathbf{S}_0}$ the set of $Q \in \mathbf{S}_0$ with $|Q| \leq \delta$). We set $K_\varepsilon := K \cap \{\phi \leq \varepsilon\}$. We integrate (2.5.12) with respect to A. We change the order of the integrations on $x \in \Omega$ and $A \in B_\delta^{\mathbf{S}_0}$ and introduce the new variable $B := u_\varepsilon(x) - A$. We obtain

$$\int_{B_\delta^{\mathbf{S}_0}} E_\varepsilon\left(u_\varepsilon^A\right) \mathrm{d}\mathscr{H}^5(A) \leq C \int_\Omega \left\{ \left(\int_{K \backslash K_\varepsilon} \frac{\mathrm{d}\mathscr{H}^5(B)}{\phi^2(B)} + \varepsilon^{-2} \mathscr{H}^5(K_\varepsilon) \right) \left|\nabla u_\varepsilon\right|^2 + \varepsilon^{-2} \mathscr{H}^5(K_\varepsilon) \right\} \mathrm{d}x.$$

We claim that

$$\mathscr{H}^5(K_\varepsilon) \leq C\varepsilon^2 \qquad \text{and} \qquad \int_{K \backslash K_\varepsilon} \frac{\mathrm{d}\mathscr{H}^5(B)}{\phi^2(B)} \leq C\left(|\log \varepsilon| + 1\right). \tag{2.5.13}$$

To simplify the presentation, we postpone the proof of these inequalities. With the help of (2.5.13), we obtain

$$\int_{B_\delta^5} E_\varepsilon\left(u_\varepsilon^A\right) \mathrm{d}\mathscr{H}^5(A) \leq C \left\{ \left(|\log \varepsilon| + 1\right) \left\|\nabla u_\varepsilon\right\|_{L^2(\Omega)}^2 + 1 \right\} \leq C\left(|\log \varepsilon| + 1\right).$$

Therefore, we can choose $A_0 \in \mathbf{S}_0$ such that $|A_0| \leq \delta$ and

$$E_\varepsilon\left(u_\varepsilon^{A_0}\right) \leq C\left(|\log\varepsilon| + 1\right). \tag{2.5.14}$$

The map $u_\varepsilon^{A_0}$ satisfies the desired energy estimate, but it does not satisfy the boundary condition, since

$$u_\varepsilon^{A_0} = \mathscr{R}\left(g_\varepsilon - A_0\right) \qquad \text{on } \partial\Omega \tag{2.5.15}$$

if ε is small enough. To correct this, we consider the maps $\left(\mathscr{R}_A\right)_{A\in B_\delta^{\mathbf{S}_0}}$ defined by

$$\mathscr{R}_A \colon Q \in \mathscr{N} \mapsto \mathscr{R}(Q - A).$$

This is a continuous family of mappings in $C^1(\mathscr{N},\, \mathscr{N})$ and $\mathscr{R}_0 = \mathrm{Id}_{\mathscr{N}}$. Therefore, when δ is small the map $\mathscr{R}_A \colon \mathscr{N} \to \mathscr{N}$ is a diffeomorphism for any $A \in B_\delta^{\mathbf{S}_0}$ (in particular for $A = A_0$). On the set

$$\mathscr{N}' := \left\{\lambda Q \colon \lambda \in \mathbb{R}^+,\ Q \in \mathscr{N}\right\},$$

we extend $\mathscr{R}_{A_0}^{-1}$ to a Lipschitz function $\mathscr{F} \colon \mathscr{N}' \to \mathscr{N}'$ by setting

$$\mathscr{F}(\lambda Q) := \lambda \mathscr{R}_{A_0}^{-1}(Q) \qquad \text{for any } \lambda \in \mathbb{R}^+,\ Q \in \mathscr{N}.$$

Remark that any $P \in \mathscr{N}' \setminus \{0\}$ can be uniquely written in the form $P = \lambda Q$ for $\lambda \in \mathbb{R}^+$ and $Q \in \mathscr{N}$, so $\mathscr{F}$ is well-defined. Also, $f \circ \mathscr{F}(P) = f(P)$ because $\mathscr{F}(P)$ and P have the same scalar invariants. The map $P_\varepsilon := \mathscr{F} \circ u_\varepsilon^{A_0}$ is well-defined, because $u_\varepsilon^{A_0} \in \mathscr{N}'$. Moreover, P_ε belongs to $H^1_{g_\varepsilon}(\Omega,\, \mathbf{S}_0)$ thanks to (2.5.15), and satisfies

$$E_\varepsilon(P_\varepsilon) \leq C\left(|\log\varepsilon| + 1\right)$$

due to (2.5.14). By comparison, the minimizers satisfy (2.5.2). □

The claim (2.5.13) follows by this

Lemma 2.5.4. *For any $R > 0$, there exist positive constants C_R, M_R such that, for any non increasing, non negative function $g \colon \mathbb{R}^+ \to \mathbb{R}^+$, there holds*

$$\int_{B_R^{\mathbf{S}_0}} (g \circ \phi)(Q)\, \mathrm{d}\mathscr{H}^5(Q) \leq C_R \int_0^{M_R} \left(s + s^4\right) g(s)\, \mathrm{d}s.$$

Assuming that the lemma holds true, choose R so large that $K \subseteq B_R^{\mathbf{S}_0}$. Then, the two assertions of Claim (2.5.13) follow by taking $g = \mathbb{1}_{(0,\,\varepsilon)}$ and $g(s) = \varepsilon^{-2}\mathbb{1}_{(0,\,\varepsilon)}(s) + s^{-2}\mathbb{1}_{[\varepsilon,\,+\infty)}(s)$, respectively. For the sake of clarity, we split the proof of Lemma 2.5.4 into a few technical results. For $r > 0$, we let dist_r denote the geodesic distance in $\partial B_r^{\mathbf{S}_0}$, that is

$$\mathrm{dist}_r(x,\, A) := \inf\left\{\int_0^1 |\gamma'(t)|\, \mathrm{d}t \colon \gamma \in C^1([0,\,1],\, \partial B_1^{\mathbf{S}_0}),\ \gamma(0) = x,\ \gamma(1) \in A\right\} \tag{2.5.16}$$

for any $x \in \partial B_r^{\mathbf{S}_0}$ and $A \subseteq \partial B_r^{\mathbf{S}_0}$, and set $\mathscr{N}'_r := \mathscr{C} \cap \partial B_r^{\mathbf{S}_0}$.

Lemma 2.5.5. *There exists a positive constant α such that*

$$\phi(Q) \geq \alpha\, \mathrm{dist}_{|Q|}\left(Q,\, \mathscr{N}'_{|Q|}\right) \qquad \textit{for any } Q \in \mathbf{S}_0.$$

Proof. The inequality holds trivially for $Q = 0$, and both sides are positively homogeneous of degree 1 (for the left-hand side we apply Lemma 2.2.3, whereas the homogeneity of the right-hand side follows directly from (2.5.16)). Thus, we can assume without loss of generality that $|Q| = 1$. By Lemma 2.2.1 and (2.2.1), the matrix Q can be written in the form

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) + sr\left(\mathbf{m}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right)$$

for some orthonormal pair $(\mathbf{n},\, \mathbf{m})$, some $r \in [0,\, 1]$ and $s := (3/2)^{1/2}$. On the other hand, any matrix $P \in \mathscr{N}_1'$ can be written as

$$P = -s\left(\mathbf{p}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right)$$

for some unit vector $\mathbf{p}$ (see Lemma 2.2.2). Through simple algebra, we obtain

$$|Q - P|^2 = \frac{2}{3}s^2\sqrt{r^2 - r + 1}\left(2\sqrt{r^2 - r + 1} - r - 1\right) + 2s^2\left((\mathbf{n}\cdot\mathbf{p})^2 + r(\mathbf{m}\cdot\mathbf{p})^2\right).$$

For each fixed $\mathbf{n}$, $\mathbf{m}$ and r, the minimum of this quantity is achieved for $\mathbf{p} = \pm\mathbf{n}\times\mathbf{m}$, therefore

$$\mathrm{dist}^2(Q,\, \mathscr{N}_1') = \frac{2}{3}s^2\sqrt{r^2 - r + 1}\left\{(1-r)^2 - \left(\sqrt{r^2 - r + 1} - 1\right)^2\right\} \leq \frac{2}{3}s^2(1-r)^2 = \frac{2}{3}s_*^2\phi^2(Q).$$

Moreover, there exists a constant C such that the inequality

$$\mathrm{dist}_1(Q,\, P) \leq C\,|Q - P|$$

holds true for any $Q,\, P \in \partial B_1^{\mathbf{S}_0}$. Then, the lemma follows. $\square$

Lemma 2.5.6. *Let $\mathscr{N}'$ be a compact n-submanifold of a smooth Riemann m-manifold $\mathscr{M}$, and let*

$$U_\delta := \{x \in \mathscr{M}\colon\ \mathrm{dist}_{\mathscr{M}}(x,\, \mathscr{N}') \leq \delta\}$$

be the δ-neighborhood of $\mathscr{N}'$ in $\mathscr{M}$, for $\delta > 0$ (here $\mathrm{dist}_{\mathscr{M}}$ stands for the geodesic distance in $\mathscr{M}$). There exist $\delta_* > 0$ and, for any $\delta \in (0,\, \delta_*)$, a constant $C = C(\mathscr{M},\, \mathscr{N}', \delta) > 0$ such that for any decreasing function $h\colon \mathbb{R}^+ \to \mathbb{R}^+$ there holds

$$\int_{U_\delta} h\left(\mathrm{dist}_{\mathscr{M}}(x,\, \mathscr{N}')\right)\,\mathrm{d}\mathscr{H}^m(x) \leq C\int_0^{C\delta} s^{m-n-1}h(s)\,\mathrm{d}s.$$

Proof. We identify $\mathbb{R}^m = \mathbb{R}^n \times \mathbb{R}^{m-n}$, and call the variable $y = (y',\, z) \in \mathbb{R}^n \times \mathbb{R}^{m-n}$. For a small $\delta_* > 0$, the δ_*-neighborhood U_{δ_*} can be covered with finitely many open sets $(V_j)_{1\leq j\leq K}$ and, for each j, there exists a bilipschitz homeomorphism $\varphi_j\colon V_j \to W_j \subseteq \mathbb{R}^m$ which maps $\mathscr{N}' \cap V_j$ onto $\mathbb{R}^n \cap W_j$. Due to the bilipschitz continuity of the φ_j's, there exist two constants γ_1, γ_2 such that, for any j and any $y = (y',\, z) \in W_j$, there holds

$$\gamma_1\,|z| \leq \mathrm{dist}_{\mathscr{M}}(\varphi_j^{-1}(y),\, \mathscr{N}) \leq \gamma_2\,|z|\,.$$

Therefore, if $0 < \delta < \delta_*$ the change of variable $x = \varphi_j^{-1}(y)$ implies

$$\begin{aligned}\int_{U_\delta} h\left(\mathrm{dist}_{\mathscr{M}}(x,\, \mathscr{N}')\right)\,\mathrm{d}\mathscr{H}^m(x) &\leq \sum_{j=1}^K \int_{\varphi_j^{-1}(V_j)} h\left(\gamma_1|z|\right)\left|\mathrm{J}\varphi_j^{-1}(y)\right|\,\mathrm{d}\mathscr{H}^m(y)\\ &\leq M\int_{B^{m-n}(0,\,\gamma_2\delta)} h(\gamma_1|z|)\,\mathrm{d}\mathscr{H}^{m-n}(z)\end{aligned}$$

where M is an upper bound for the norm of the Jacobians $\mathrm{J}\varphi_j^{-1}$. Then, passing to polar coordinates,

$$\begin{aligned}\int_{U_\delta} h\left(\mathrm{dist}_{\mathscr{M}}(x,\, \mathscr{N}')\right)\,\mathrm{d}\mathscr{H}^m(x) &\leq M\int_0^{\gamma_2\delta} \rho^{m-n-1}h(\gamma_1\rho)\,\mathrm{d}\rho\\ &\leq M\gamma_1^{1+n-m}\int_0^{\gamma_1\gamma_2\rho} s^{m-n-1}h(s)\,\mathrm{d}s.\end{aligned}$$ $\square$

Proof of Lemma 2.5.4. By Lemma 2.2.3, the function ϕ is positively homogeneous of degree 1. Then,

$$\int_{B_R^{\mathbf{S}_0}} (g \circ \phi)(Q)\, \mathrm{d}\mathscr{H}^5(Q) = \int_0^R \rho^4 \int_{\partial B_1^{\mathbf{S}_0}} g\left(\rho\phi(Q)\right)\, \mathrm{d}\mathscr{H}^4(Q)\, \mathrm{d}\rho.$$

By applying Lemma 2.5.5, and since g is a decreasing function,

$$\int_{B_R^{\mathbf{S}_0}} (g \circ \phi)(Q)\, \mathrm{d}\mathscr{H}^5(Q) \leq \int_0^R \rho^4 \int_{\partial B_1^{\mathbf{S}_0}} g\left(\alpha\rho \operatorname{dist}_1(Q,\, \mathscr{N}_1')\right)\, \mathrm{d}\mathscr{H}^4(Q)\, \mathrm{d}\rho.$$

Now, we apply Lemma 2.5.6 with $\mathscr{M} = \partial B_1^{\mathbf{S}_0}$, $\mathscr{N}' = \mathscr{N}_1'$ and $h\colon s \mapsto g(\alpha\rho s)$. We find constants δ and C such that, letting U_δ be the δ-neighborhood of $\mathscr{N}_1'$ in $\partial B_1^{\mathbf{S}_0}$ and $V_\delta := \partial B_1^{\mathbf{S}_0} \setminus U_\delta$, we have

$$\begin{aligned}
&\int_{B_R^{\mathbf{S}_0}} (g \circ \phi)(Q)\, \mathrm{d}\mathscr{H}^5(Q) \\
&\qquad = \int_0^R \rho^4 \left\{ \int_{U_\delta} g\left(\alpha\rho \operatorname{dist}_1(Q,\, \mathscr{N}_1')\right)\, \mathrm{d}\mathscr{H}^4(Q) + \int_{V_\delta} g\left(\alpha\rho \operatorname{dist}_1(Q,\, \mathscr{N}_1')\right)\, \mathrm{d}\mathscr{H}^4(Q) \right\} \mathrm{d}\rho \\
&\qquad \leq C \int_0^R \rho^4 \left\{ \int_0^{C\delta} s g(\alpha\rho s)\, \mathrm{d}s + g(\alpha\rho\delta)\, \mathscr{H}^4(V_\delta) \right\} \mathrm{d}\rho
\end{aligned}$$

(to bound the integral on V_δ, we use again that g is decreasing). Now, the two terms can be easily handled by changing the variables and using Fubini-Tonelli theorem:

$$\begin{aligned}
\int_{B_R^{\mathbf{S}_0}} (g \circ \phi)(Q)\, \mathrm{d}\mathscr{H}^5(Q) &\leq \alpha^{-2} C \int_0^R \rho^2 \int_0^{\alpha\rho\delta C} t g(t)\, \mathrm{d}t\, \mathrm{d}\rho + (\alpha\delta)^{-5} C \mathscr{H}^4(V_\delta) \int_0^{\alpha\delta R} t^4 g(t)\, \mathrm{d}t \\
&\leq C_{\alpha,\delta,R} \int_0^{C_{\alpha,\delta,R}} \left(t + t^4\right) g(t)\, \mathrm{d}t.
\end{aligned}$$

Since α, δ depend only on ϕ, $\mathscr{N}_1'$, the lemma is proved. □

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La solution à symétrie radiale du modèle de Landau-de Gennes dans une couronne en dimension trois

Nous nous intéressons à la stabilité du hérisson radiale dans une couronne en dimension 3, en imposant des conditions au bord à symétrie radiale, dans le cadre de la théorie de Landau-de Gennes pour les phases nématiques. Nous montrons que le hérisson est l'unique minimiseur dans les deux cas suivants : (i) si la largeur de la couronne est suffisamment petite, dès que la température est suffisamment basse pour empêcher les phénomènes de surfusion ; (ii) dans le régime des très basses températures, pour une couronne de n'importe quelle largeur. Dans le cas (i), nous donnons une condition explicite, en termes de la largeur de la couronne, pour la minimalité du hérisson.

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Chapter 3

Radial symmetry on three-dimensional shells in the Landau-de Gennes theory

Joint work with Apala Majumdar[1] and Mythily Ramaswamy[2].

[1] Department of Mathematical Sciences, University of Bath, Bath, United Kingdom

[2] TIFR-CAM, Bangalore, India

Abstract

We study the stability of the radial-hedgehog solution on a three-dimensional spherical shell with radial boundary conditions, within the Landau-de Gennes theory for nematic liquid crystals. We show that the radial-hedgehog solution has no zeros for a sufficiently narrow shell, for all temperatures below the nematic supercooling temperature. We prove that the radial-hedgehog solution is the unique global Landau-de Gennes energy minimizer for this problem in two separate cases: (i) a sufficiently narrow shell, for all temperatures below the nematic supercooling temperature, (ii) the low temperature limit, for all values of the shell width. In case (i), we provide explicit geometry-dependent criteria for the global minimality of the radial-hedgehog solution.

Contents

Keywords. Radially symmetric solutions, nematic liquid crystals, Landau-de Gennes theory, radial-hedgehog, minimizing configurations, stable configurations.

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3.1 Introduction

Nematic liquid crystals are anisotropic liquids with long-range orientational ordering i.e. liquids with distinguished directions [38, 108]. Continuum theories for nematics e.g. Oseen-Frank, Ericksen and Landau-de Gennes theories, have received considerable attention in the mathematical literature [44, 60, 87], of which the Landau-de Gennes theory is the most general. The Landau-de Gennes theory is popular in the context of studying intricate defect patterns in nematic textures. However, it is remarkable that the Landau-de Gennes theory predicts no analytic singularities for the corresponding equilibria and a rigorous mathematical description of defects in the Landau-de Gennes framework is missing to date.

The radial-hedgehog solution is the classical example of a point defect in the liquid crystal literature [38, 140]. The radial-hedgehog solution has a disordered "isotropic" defect core and the molecules point radially outwards everywhere away from the defect core. There are several mathematical analogies between the Landau-de Gennes theory for nematic liquid crystals and the Ginzburg-Landau theory of superconductivity. The radial-hedgehog solution is analogous to the degree +1-vortex in the Ginzburg-Landau theory. The degree +1-vortex is a well studied solution in the Ginzburg-Landau community [14, 100, 113]. In fact, in [100, 113], the authors prove that the degree +1-vortex solution is the unique solution (up to translation and rotation) of the Ginzburg-Landau equations on $\mathbb{R}^3$, subject to certain natural energy bounds and topologically non-trivial boundary conditions. In [100, 113], the authors derive this powerful symmetry result for the system of Ginzburg-Landau equations for three-dimensional vectors on $\mathbb{R}^3$ i.e. maps $\mathbf{u}\colon \mathbb{R}^3 \to \mathbb{R}^3$, or more generally, N-dimensional vectors defined on $\mathbb{R}^N$. When we work with the Landau-de Gennes theory for nematics, we study a nonlinear coupled system of partial differential equations for a five-dimensional tensor-valued $\mathbf{Q}$-order parameter defined on a three-dimensional domain i.e. we study maps, $\mathbf{Q}\colon \Omega \subseteq \mathbb{R}^3 \to \mathbb{R}^5$. There are two additional degrees of freedom which can drastically alter the solution landscape in spite of apparent mathematical similarities between the Landau-de Gennes system and the Ginzburg-Landau system [71, 98]. For example, it is known that the radial-hedgehog solution loses stability with respect to biaxial (higher-dimensional) perturbations on a three-dimensional spherical droplet with radial boundary conditions, for low temperatures, within the Landau-de Gennes theory for nematics, see [51, 71, 96, 132]. The geometry and the boundary conditions enforce the radial-hedgehog solution to have an "isotropic" core at the droplet center and the isotropic core is energetically expensive for low temperatures. The global energy minimizer has a biaxial defect core localized near the droplet center and the radial-hedgehog solution describes the approximate far-field behaviour of the global energy minimizer, away from the biaxial defect core, in some asymptotic limits.

We re-visit the problem of the radial-hedgehog solution within the Landau-de Gennes theory, on a 3D spherical shell with Dirichlet radial boundary conditions on both the inner and outer spherical surfaces. In effect, we study the effect of excluding the origin from the spherical domain, whilst imposing the Dirichlet radial boundary conditions. Stemming from Nelson's seminal paper [111], the nematic equilibrium texture on spherical shells has being driven attention both from the physical and numerical point of view (see, for instance, [141] and [52]). In the literature, boundary data are usually assumed to be tangent to boundary of the shell, whereas we take radial boundary data because we are interested in the radial symmetry of solutions. Within this framework, we are able to prove rigorously the global minimality of the radial-hedgehog. Although it may seem physically intuitive, this result is not obvious from a mathematical point of view, especially since it is known that the radial solution is not always a minimizer for the Ginzburg-Landau functional on a 2D annulus [54].

The radial-hedgehog solution is defined by a scalar order parameter, h_t, which vanishes at isotropic points [71, 96]. Firstly, we show that the radial-hedgehog solution, defined to be a minimizer of an appropriately defined functional, has no isotropic/zero points on a 3D spherical shell, for all temperatures below the nematic supercooling temperature. In fact, we can use either the width of the shell or the temperature to control the magnitude of the scalar order parameter. We emphasize that we do not consider the case of vanishing elastic constant here as this case can be dealt with by the results in [98]. In the limit of vanishing elastic constant, one can prove that minimizers of a relatively simple Landau-de Gennes energy converge uniformly to the radial-hedgehog solution on a 3D spherical shell, with two concentric spherical boundaries and Dirichlet radial conditions, by appealing to the results in [98]. In this chapter, we focus on the interplay between geometry and temperature. In Section 3.3, we compute an explicit lower bound for the scalar order parameter, h_t, as a function of the shell width, independent of the temperature. We use this bound to provide explicit geometry-dependent criteria for the local stability of the radial-hedgehog solution, for all temperatures below the critical nematic supercooling temperature. We prove the local stability by using a Hardy-type inequality to prove the positivity of the second variation of the Landau-de Gennes energy, for a sufficiently narrow 3D shell. In Section 3.4, we prove our first main result.

Theorem 3.1.1. *Let* $\Omega = \left\{x \in \mathbb{R}^3 \colon 1 \leq |x| \leq R\right\}$ *and*

$$R < \min\left\{R_0 := \exp\left(\frac{4\pi^2}{23}\right),\, R^*\right\} \tag{3.1.1}$$

where R^* is defined in Proposition 3.3.1. Then the radial-hedgehog solution is the unique global minimizer of the Landau-de Gennes problem (LG_t) *in the admissible class $\mathscr{A}$ defined in (3.2.5), for all temperatures below the critical nematic supercooling temperature.*

In addition to the positivity of the second variation, a key ingredient of Theorem 3.1.1 is a quantitative control on the non-quadratic terms in the Landau-de Gennes energy density. We prove that the non-quadratic contributions are non-negative for $h_t \simeq 1$ and this suffices to establish Theorem 3.1.1. The smallness condition on $R-1$ ensures the positivity of the quadratic terms, via a good Poincaré constant, but is is also crucial for estimating the non-quadratic terms, because it implies a good control from below on the scalar order parameter h_t, via the results of Section 3.3.

In Section 3.5, we study the effect of the reduced temperature, t, on the stability of the radial-hedgehog solution. In particular, $t = 0$ corresponds to the nematic supercooling temperature. We show that t can be used to control the magnitude of the scalar order parameter, h_t, and use this control to demonstrate the local stability of the radial-hedgehog solution, for all values of the shell width, for sufficiently large values of t. Our second main result concerns the global minimality of the radial-hedgehog solution in the $t \to \infty$ limit.

Theorem 3.1.2. *Let $\Omega \subseteq \mathbb{R}^3$ be a 3D spherical shell as defined above. For any $R \geq 1$, there exists $\tau = \tau(R) \geq 1$ such that, for any temperature $t \geq \tau$, the radial-hedgehog is the unique global minimizer for Problem* (LG_t)*.*

As in the proof of Theorem 3.1.1, the key ingredients of Theorem 3.1.2 are an improved lower bound for the second variation of the Landau-de Gennes energy and careful manipulations of the non-quadratic components of the energy density. These manipulations are necessarily different to the control of the non-quadratic energy density terms in Theorem 3.1.1 but both approaches heavily rely on controlling the magnitude of the scalar order parameter. The lower bound on the second variation is deduced from recent results of Ignat et al. [73], where the authors prove local stability of the hedgehog in the whole space $\mathbb{R}^3$ for $t \ll 1$.

To sum up, our proofs rely on two main elements: positivity of the second variation and a good pointwise control on the scalar order parameter h_t. This information allow us to prove rigorous local stability and global minimality results. Hence, we believe that our work has wider scope in analytically understanding how the various quadratic and non-quadratic components of the Landau-de Gennes energy density quantitatively compete and contribute to the solution energies.

3.2 Preliminaries

We work within the Landau-de Gennes theory for nematic liquid crystals wherein the nematic configuration is described by the **Q**-tensor [4] order parameter [38]. The **Q**-tensor mathematically corresponds to

4. For the sake of clarity, throughout the chapter bold symbols will be used to denote tensors.

a symmetric, traceless 3×3 matrix. Let $\mathbf{S}_0$ denote the space of all symmetric, traceless 3×3 matrices defined by

$$\mathbf{S}_0 := \{\mathbf{Q} \in \mathrm{M}_3(\mathbb{R})\colon \mathbf{Q}_{ij} = \mathbf{Q}_{ji},\ \mathbf{Q}_{ii} = 0,\ i,j = 1,2,3\}.$$

The domain is a 3D spherical shell, with outer radius R and inner radius set to unity, as shown below

$$\Omega := \left\{x \in \mathbb{R}^3\colon 1 \le |x| \le R\right\} \quad \text{where} \quad R > 1.$$

A $\mathbf{Q}$-tensor is said to be (i) isotropic when $\mathbf{Q} = 0$, (ii) uniaxial when $\mathbf{Q}$ has two degenerate non-zero eigenvalues and (iii) biaxial when $\mathbf{Q}$ has three distinct eigenvalues [38, 140]. A uniaxial $\mathbf{Q}$-tensor can be written in the form

$$\mathbf{Q}_u = s\left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{Id}}{3}\right)$$

for a real-valued order parameter, s, and a unit-vector field $\mathbf{n} \in \mathbb{S}^2$ i.e. $\mathbf{Q}_u$ has three degrees of freedom whereas a biaxial $\mathbf{Q}$-tensor uses all five degrees of freedom. In physical terms, a uniaxial $\mathbf{Q}$-tensor corresponds to a nematic configuration with a single distinguished direction of molecular alignment whereas a biaxial $\mathbf{Q}$-tensor corresponds to a configuration with two preferred directions of molecular alignment.

We consider a simple form of the Landau-de Gennes energy given by [38, 108]

$$F(\mathbf{Q}) := \int_\Omega \left\{\frac{L}{2}|\nabla \mathbf{Q}|^2 + f_B(\mathbf{Q})\right\}.$$

In what follows, we assume that the elastic constant $L > 0$ is fixed once and for all, e.g., $L = 1$ (Newton), since the $L \to 0$ limit has been well-studied in recent years [98]. We use Einstein summation convention throughout the notes i.e. $|\nabla \mathbf{Q}|^2 = \mathbf{Q}_{ij,k}\mathbf{Q}_{ij,k}$ and $i,\ j,\ k = 1,\ 2,\ 3$. The bulk potential, f_B, drives the nematic-isotropic phase transition and for the our purposes, we take f_B to be a quartic polynomial in the $\mathbf{Q}$-tensor invariants as shown below:

$$f_B(\mathbf{Q}) := \frac{A}{2}\operatorname{tr}\mathbf{Q}^2 - \frac{B}{3}\operatorname{tr}\mathbf{Q}^3 + \frac{C}{4}\left(\operatorname{tr}\mathbf{Q}^2\right)^2,$$

where $\operatorname{tr}\mathbf{Q}^2 = \mathbf{Q}_{ij}\mathbf{Q}_{ij}$, $\operatorname{tr}\mathbf{Q}^3 = \mathbf{Q}_{ij}\mathbf{Q}_{jp}\mathbf{Q}_{pi}$ and $i,\ j,\ p$ range in $\{1,\ 2,\ 3\}$. The coefficient A depends on the material and the temperature, as $A = \alpha(T - T^*)$ where $\alpha > 0$ is a material-dependent constant, T is the temperature and T^* is the critical nematic supercooling temperature [95, 108]. We work with temperatures $T \le T^*$, so that $A \le 0$, and we treat $B,\ C > 0$ to be fixed material-dependent constants.

For $A \le 0$, a standard computation (see [95]) shows that f_B attains its minimum on the set of *uniaxial* $\mathbf{Q}$-tensors given by

$$\mathscr{N} := \left\{s_*\left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{Id}}{3}\right) : n \in \mathbb{S}^2\right\}, \tag{3.2.1}$$

where

$$s_* := \frac{B + \sqrt{B^2 + 24|A|C}}{4C}.$$

We introduce the scalings

$$t := \frac{27|A|C}{B^2}, \qquad \lambda(t) := \frac{3 + \sqrt{9 + 8t}}{4}, \qquad \bar{L} := \frac{27CL}{2B^2}$$

$$\bar{x} := \frac{x}{\sqrt{\bar{L}}}, \qquad \bar{\mathbf{Q}} := \frac{1}{s_*}\sqrt{\frac{3}{2}}\mathbf{Q}.$$

One can easily verify that

$$s_* = \frac{B}{3C}\lambda(t), \quad 2\lambda(t)^2 = 3\lambda(t) + t.$$

In what follows, we refer to t as the reduced temperature and always work with $t \geq 0$. The re-scaled domain is

$$\bar{\Omega} = \left\{ x \in \mathbb{R}^3 \colon \frac{1}{\sqrt{\bar{L}}} \leq |\bar{x}| \leq \frac{R}{\sqrt{\bar{L}}} \right\}. \tag{3.2.2}$$

We measure the dimensionless length in units of $\bar{L}^{-1/2}$ and hence (3.2.2) is equivalent to

$$\bar{\Omega} = \left\{ x \in \mathbb{R}^3 \colon 1 \leq |\bar{x}| \leq R \right\}$$

where $R > 1$ is the dimensionless outer radius. We drop the *bars* in what follows and all statements are to be understood in terms of the re-scaled variables. The re-scaled Landau-de Gennes functional is given by

$$F_t(\mathbf{Q}) := \int_\Omega \left\{ \frac{1}{2}|\nabla \mathbf{Q}|^2 + \frac{t}{8}\left(1 - |\mathbf{Q}|^2\right)^2 + \frac{\lambda(t)}{8}\left(1 - 4\sqrt{6}\,\mathrm{tr}\,\mathbf{Q}^3 + 3|\mathbf{Q}|^4\right) \right\}. \tag{3.2.3}$$

The re-scaled bulk potential corresponds to $f_B(\mathbf{Q}) - \min_{\mathbf{Q}\in\mathbf{S}_0} f_B(\mathbf{Q})$, where we have introduced an additive constant to make the bulk energy density non-negative. We impose Dirichlet radial boundary conditions on the inner and outer radii as shown below:

$$\mathbf{Q} = \mathbf{Q}_b \quad \text{on } r = 1 \text{ and } r = R \tag{3.2.4}$$

where

$$\mathbf{Q}_b := \sqrt{\frac{3}{2}}\left(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}} - \frac{\mathbf{Id}}{3} \right).$$

The unit-vector, $\hat{\mathbf{x}} := \frac{x}{r}$ with $r := |x|$, is the radial unit-vector. By definition, $\mathbf{Q}_b$ is perfectly uniaxial and is a minimum of the bulk potential, i.e., it takes its values in the set defined by (3.2.1).

We study the variational problem

$$\min_{\mathbf{Q}\in\mathscr{A}} F_t(\mathbf{Q}), \tag{LG$_t$}$$

where F_t is given by (3.2.3) and $\mathscr{A}$ is the admissible class defined by

$$\mathscr{A} := \left\{ \mathbf{Q} \in W^{1,2}(\Omega, \mathbf{S}_0) : \mathbf{Q} = \mathbf{Q}_b \quad \text{on } r = 1 \text{ and } r = R \right\}. \tag{3.2.5}$$

The corresponding Euler-Lagrange equations are given by

$$\Delta \mathbf{Q}_{ij} = \frac{t}{2}\mathbf{Q}_{ij}\left(|\mathbf{Q}|^2 - 1\right) + \frac{\lambda(t)}{8}\left(12|\mathbf{Q}|^2\mathbf{Q}_{ij} - 12\sqrt{6}\mathbf{Q}_{ip}\mathbf{Q}_{pj} + 4\sqrt{6}|\mathbf{Q}|^2\delta_{ij}\right). \tag{3.2.6}$$

We are interested in *locally stable* equilibria, that is, solutions of (3.2.6) for which the second variation of F_t is positive (see Subsection 3.3.2 and Section 3.5), including minimizers for the problem (LG$_t$).

3.3 The radial-hedgehog solution

We define the radial-hedgehog solution to be a minimizer of the Landau-de Gennes energy (3.2.3) in the class of all radially-symmetric uniaxial $\mathbf{Q}$-tensors. This is analogous to the definition of the radial-hedgehog solution on a 3D spherical droplet with radial boundary conditions, as previously used in the literature [71, 96, 132].

We define the radial-hedgehog solution to be

$$\mathbf{H}_t := \sqrt{\frac{3}{2}} h_t(r) \left(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}} - \frac{\mathbf{Id}}{3} \right) \tag{3.3.1}$$

where $h_t(r)$ is a minimizer of

$$E(h_t) := \int_1^R \left\{ \frac{r^2}{2}\left(\frac{\mathrm{d}h}{\mathrm{d}r}\right)^2 + 3h^2 + \frac{tr^2}{8}(1-h^2)^2 + \frac{\lambda(t)r^2}{8}\left(1-4h^3+3h^4\right)\right\} \mathrm{d}r \tag{3.3.2}$$

subject to the boundary conditions

$$h_t(1) = h_t(R) = 1. \tag{3.3.3}$$

This is consistent with the Dirichlet conditions defined in (3.2.4). The admissible space for the variational problem in (3.3.2) is taken to be

$$\mathscr{A}_h := \left\{ h \in L^2\left([1,\, R],\, \mathrm{d}r\right) : \frac{\mathrm{d}h}{\mathrm{d}r} \in L^2\left([1,\, R],\, r^2\mathrm{d}r\right) \text{ s.t. } h(1) = h(R) = 1 \right\}.$$

The minimizing function $h_t \in \mathscr{A}_h$ is a solution of the following second-order ordinary differential equation

$$\frac{\mathrm{d}^2 h_t}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}h_t}{\mathrm{d}r} - \frac{6h_t}{r^2} = \frac{t}{2}h_t(h_t^2-1) + \frac{3\lambda(t)}{2}\left(h_t^3 - h_t^2\right) \tag{3.3.4}$$

subject to (3.3.3). One can check that $\mathbf{H}_t$ thus defined is a solution of the Euler-Lagrange equations in (3.2.6), i.e. $\mathbf{H}_t$ is a critical point of the Landau-de Gennes energy. In the subsequent sections, we investigate the local and global stability of $\mathbf{H}_t$ as a function of the shell width $R-1$ and the reduced temperature t.

Proposition 3.3.1. *Define the function $\eta\colon [1,\, R] \to \mathbb{R}$ to be*

$$\eta(r) = \frac{1}{R^5-1}\left((R^3-1)r^2 + (R^2-1)\left(\frac{R}{r}\right)^3 \right). \tag{3.3.5}$$

Then η satisfies the following ordinary differential equation:

$$\frac{\mathrm{d}^2\eta}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}\eta}{\mathrm{d}r} - 6\frac{\eta}{r^2} = 0 \tag{3.3.6}$$

subject to the boundary conditions $\eta(1) = \eta(R) = 1$. There exists a $R^* > 1$ such that

$$\eta(r) \geq \frac{2}{3} \quad \textit{for} \quad 1 \leq r \leq R \leq R^*.$$

Proof. One can check by substitution that η, as defined in (3.3.5), is indeed a solution of (3.3.6), subject to $\eta(1) = \eta(R) = 1$. One can compute the minimum of η as a function of R: an elementary computation shows that

$$\begin{aligned}\min_{1\leq r\leq R}\eta(r) &= \frac{5}{2^{2/5}3^{3/5}} \cdot \frac{R^{6/5}(R^2-1)^{2/5}\left(R^3-1\right)^{3/5}}{(R^5-1)} \\ &= \frac{5}{2^{2/5}3^{3/5}} \cdot \frac{R^{6/5}\left(R+1\right)^{2/5}\left(R^2+R+1\right)^{3/5}}{R^4+R^3+R^2+R+1} \xrightarrow[R\to 1]{} 1,\end{aligned}$$

so there exists $R^* > 1$ such that

$$\eta(r) \geq \frac{2}{3} \qquad \text{for } 1 \leq r \leq R,$$

when $1 < R < R^*$. $\square$

Proposition 3.3.2. *The function η, defined in* (3.3.5)*, is a lower bound for $h_t\colon [1,\, R] \to \mathbb{R}$ defined in* (3.3.1)–(3.3.4)*, i.e.,*

$$\frac{2}{3} \le \eta(r) \le h_t(r) \le 1 \quad \textit{for} \quad 1 \le r \le R \le R^*.$$

Proof. The proof is analogous to the proof in the two-dimensional case, presented in [54]. We define the function

$$\nu(r) := \eta(r) - h_t(r) \quad \text{for} \quad 1 \le r \le R$$

where $\nu(1) = \nu(R) = 0$. We proceed by contradiction. We assume that ν has a positive maximum for $r^* \in (1,\, R)$. The function ν is a solution of the following second-order differential equation

$$\frac{\mathrm{d}^2\nu}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}\nu}{\mathrm{d}r} - 6\frac{\nu}{r^2} = \frac{t}{2L}h_t(1-h_t^2) + \frac{3\lambda(t)}{2L}\left(h_t^2 - h_t^3\right). \tag{3.3.7}$$

The function h_t satisfies the bounds $0 \le h_t(r) \le 1$; these bounds are established in [71, 95]. Therefore, the right-hand side of (3.3.7) is non-negative for all $1 \le r \le R$. At $r^* \in t(1,\, R)$, we have

$$\frac{\mathrm{d}^2\nu}{\mathrm{d}r^2}|_{r=r^*} = 6\frac{\nu(r^*)}{r^{*2}} + \frac{t}{2L}h_t(1-h_t^2) + \frac{3\lambda(t)}{2L}\left(h_t^2 - h_t^3\right). \tag{3.3.8}$$

By assumption, $\nu(r^*) > 0$, so that the right-hand side of (3.3.8) is strictly positive whereas the left-hand side is non-positive by definition of a maximum point.This yields the desired contradiction and we conclude that

$$\nu(r) = \eta(r) - h_t(r) \le 0 \quad \text{for} \quad 1 \le r \le R$$

as required. ☐

3.3.1 Energy expansion

We want to study the local and global stability of the radial-hedgehog solution, $\mathbf{H}_t$ defined in (3.3.1), in the admissible space $\mathscr{A}$ defined by (3.2.5). Let $\mathbf{Q} \in \mathscr{A}$ be an arbitrary $\mathbf{Q}$-tensor in our admissible space. Then $\mathbf{Q}$ can be written as

$$\mathbf{Q}_{ij} = \mathbf{H}_{t,ij} + \mathbf{V}_{ij} \quad \text{for} \quad i,j = 1,2,3$$

with $\mathbf{V} \in W^{1,2}\left(\Omega,\, \mathbf{S}_0\right)$ and

$$\mathbf{V} = 0 \quad \text{on } r = 1 \text{ and } r = R,$$

since $\mathbf{Q} - \mathbf{H}_t = 0$ on the boundaries. The first step is to compute an energy expansion for $\mathbf{Q}$ in terms of $\mathbf{H}_t$ and $\mathbf{V}$; a straightforward computation shows that

$$\begin{aligned}
|\mathbf{Q}|^2 &= h_t^2 + 2\left(\mathbf{H}_t \cdot \mathbf{V}\right) + |\mathbf{V}|^2 \\
|\mathbf{Q}|^4 &= h_t^4 + 4h_t^2\left(\mathbf{H}_t \cdot \mathbf{V}\right) + 2h_t^2|\mathbf{V}|^2 + 4\left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 + 4(\mathbf{H}_t \cdot \mathbf{V})|\mathbf{V}|^2 + |\mathbf{V}|^4 \\
\left(1 - |\mathbf{Q}|^2\right)^2 &= \left(1 - h_t^2\right)^2 + 4\left(\mathbf{H}_t \cdot \mathbf{V}\right)\left(h_t^2 - 1\right) + 2|\mathbf{V}|^2\left(h_t^2 - 1\right) + 4\left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 + 4\left(\mathbf{H}_t \cdot \mathbf{V}\right)|\mathbf{V}|^2 + |\mathbf{V}|^4 \\
\operatorname{tr}\mathbf{Q}^3 &= \frac{h_t^3}{\sqrt{6}} + 3\operatorname{tr}\left(\mathbf{H}_t^2\mathbf{V} + \mathbf{H}_t\mathbf{V}^2\right) + \operatorname{tr}\mathbf{V}^3 \\
|\nabla\mathbf{Q}|^2 &= \left|\nabla\mathbf{H}_t\right|^2 + 2\left(\nabla\mathbf{H}_t \cdot \nabla\mathbf{V}\right) + \left|\nabla\mathbf{V}\right|^2.
\end{aligned}$$

We note that

$$\operatorname{tr}(\mathbf{H}_t\mathbf{V}^2) = \sqrt{\frac{3}{2}}h_t\left(r\right)\left(\left(\hat{\mathbf{x}} \cdot \mathbf{V}\right)^2 - \frac{|\mathbf{V}|^2}{3}\right).$$

The Landau-de Gennes energy of $\mathbf{Q}$ can then be written as

$$
\begin{aligned}
F_t(\mathbf{Q}) = F_t(\mathbf{H}_t) &+ \int_\Omega \left\{ \nabla \mathbf{H}_t \cdot \nabla \mathbf{V} + \frac{t}{2} \left(\mathbf{H}_t \cdot \mathbf{V}\right) \left(h_t^2 - 1\right) \right\} \\
&+ \int_\Omega \frac{\lambda(t)}{8} \left(12 h_t^2 \left(\mathbf{H}_t \cdot \mathbf{V}\right) - 12\sqrt{6}\, \mathrm{tr}\left(\mathbf{H}_t^2 \mathbf{V}\right) \right) \\
&+ \int_\Omega \left\{ \frac{1}{2} |\nabla \mathbf{V}|^2 + \frac{t}{8} \left(4 \left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 + 2 |\mathbf{V}|^2 \left(h_t^2 - 1\right) \right) \right\} \\
&+ \int_\Omega \frac{\lambda(t)}{8} \left(6 h_t^2 |\mathbf{V}|^2 + 12 \left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 - 12\sqrt{6}\, \mathrm{tr}\left(\mathbf{H}_t \mathbf{V}^2\right) \right) \\
&+ \int_\Omega \left\{ \frac{t}{2} \left(\mathbf{H}_t \cdot \mathbf{V}\right) |\mathbf{V}|^2 + \frac{\lambda(t)}{8} \left(12 \left(\mathbf{H}_t \cdot \mathbf{V}\right) |\mathbf{V}|^2 - 4\sqrt{6}\, \mathrm{tr}\, \mathbf{V}^3 \right) \right\} \\
&+ \int_\Omega \left\{ \frac{t}{8} |\mathbf{V}|^4 + \frac{3\lambda(t)}{8} |\mathbf{V}|^4 \right\}.
\end{aligned} \tag{3.3.9}
$$

The sum of the first and the second line (that is, all the linear terms in $\mathbf{V}$) vanishes since $\mathbf{H}_t$ is a critical point of the Landau-de Gennes energy.

We use the following basis for the space $\mathbf{S}_0$, as introduced in [73]. Let $\mathbf{n} = \hat{\mathbf{x}}$ and let $(\mathbf{n}, \mathbf{m}, \mathbf{p})$ denote an orthonormal basis for $\mathbb{R}^3$. In terms of spherical polar coordinates (r, θ, ϕ), we have

$$
\begin{aligned}
\mathbf{n} &:= (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \\
\mathbf{m} &:= (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta) \\
\mathbf{p} &:= (-\sin\phi, \cos\phi, 0)
\end{aligned}
$$

for $0 \leq \theta \leq \pi$, $0 \leq \phi < 2\pi$. Following the paradigm in [73], we define

$$
\mathbf{E} := \mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{Id}}{3}, \qquad \mathbf{F} := \mathbf{n} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{n}, \qquad \mathbf{G} := \mathbf{n} \otimes \mathbf{p} + \mathbf{p} \otimes \mathbf{n}
$$
$$
\mathbf{X} := \mathbf{m} \otimes \mathbf{p} + \mathbf{p} \otimes \mathbf{m}, \qquad \mathbf{Y} := \mathbf{m} \otimes \mathbf{m} - \mathbf{p} \otimes \mathbf{p}
$$

where $|\mathbf{E}|^2 = 2/3$ and $|\mathbf{F}|^2 = |\mathbf{G}|^2 = |\mathbf{X}|^2 = |\mathbf{Y}|^2 = 2$. Then any arbitrary $\mathbf{V} \in \mathbf{S}_0$ can be written as

$$
\mathbf{V} = v_0 \mathbf{E} + v_1 \mathbf{F} + v_2 \mathbf{G} + v_3 \mathbf{X} + v_4 \mathbf{Y} \tag{3.3.10}
$$

for functions $v_0, v_1, v_2, v_3, v_4 \colon \Omega \to \mathbb{R}$ and all five functions vanish on $r = 1$ and $r = R$. The key quantities in (3.3.9) can be written in terms of $v_0, v_1, \ldots, v_4$ as shown below:

$$
|\mathbf{V}|^2 = \frac{2}{3} v_0^2 + 2\left(v_1^2 + v_2^2 + v_3^2 + v_4^2\right), \qquad \left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 = \frac{2}{3} h_t^2 v_0^2
$$

$$
\begin{aligned}
\mathbf{n}_i \mathbf{V}_{ij} &= \frac{2 v_0}{3} \mathbf{n}_j + v_1 \mathbf{p}_j + v_2 \mathbf{m}_j \\
\mathbf{m}_i \mathbf{V}_{ij} &= \left(v_4 - \frac{v_0}{3} \right) \mathbf{m}_j + v_1 \mathbf{n}_j + v_3 \mathbf{p}_j \\
\mathbf{p}_i \mathbf{V}_{ij} &= v_2 \mathbf{n}_j + v_3 \mathbf{m}_j - \left(\frac{v_0}{3} + v_4 \right) \mathbf{p}_j
\end{aligned}
$$

and

$$
\begin{aligned}
\mathrm{tr}\, \mathbf{V}^3 &= \frac{2}{9} v_0^3 + v_0 \left(v_1^2 + v_2^2\right) + 6 v_1 v_2 v_3 + 3 v_4 \left(v_2^2 - v_1^2\right) - 2 v_0 \left(v_3^2 + v_4^2\right) \\
|\mathbf{V}|^4 &= \frac{4}{9} v_0^4 + 4\left(v_1^2 + v_2^2\right)^2 + 4\left(v_3^2 + v_4^2\right)^2 + 8\left(v_1^2 + v_2^2\right)\left(v_3^2 + v_4^2\right) + \frac{8}{3} v_0^2 \left(v_1^2 + v_2^2 + v_3^2 + v_4^2\right).
\end{aligned}
$$

Therefore, the energy difference $F_t(\mathbf{Q}) - F_t(\mathbf{H}_t)$ is

$$
\begin{aligned}
F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) = & \int_\Omega \left\{ \frac{1}{2}|\nabla \mathbf{V}|^2 + \frac{t}{4}|\mathbf{V}|^2 \left(h_t^2 - 1\right) + \frac{t}{3} h_t^2 v_0^2 \right\} \\
& + \frac{\lambda(t)}{2} \int_\Omega \left\{ \left(3h_t^2 - 2h_t\right) v_0^2 + 3\left(h_t^2 + 2h_t\right)\left(v_3^2 + v_4^2\right) + 3\left(h_t^2 - h_t\right)\left(v_1^2 + v_2^2\right) \right\} \\
& + \left(\frac{t}{\sqrt{6}} + \sqrt{\frac{3}{2}}\lambda(t) \right) \int_\Omega h_t v_0 \left(\frac{2}{3} v_0^2 + 2v_1^2 + 2v_2^2 + 2v_3^2 + 2v_4^2 \right) \\
& - \frac{\sqrt{6}}{2}\lambda(t) \int_\Omega \left\{ \frac{2}{9} v_0^3 + v_0\left(v_1^2 + v_2^2\right) + 6v_1v_2v_3 + 3v_4\left(v_1^2 - v_2^2\right) - 2v_0\left(v_3^2 + v_4^2\right) \right\} \\
& + \frac{t + 3\lambda(t)}{8} \int_\Omega \left\{ \frac{4}{9} v_0^4 + 4\left(v_1^2 + v_2^2 + v_3^2 + v_4^2\right)^2 + \frac{8}{3} v_0^2 \left(v_1^2 + v_2^2 + v_3^2 + v_4^2\right) \right\}.
\end{aligned}
$$

3.3.2 Local stability

We compute the second variation of the Landau-de Gennes energy (3.2.3) about the radial-hedgehog solution, $\mathbf{H}_t$ (defined in (3.3.1)–(3.3.4)). We recall that the second variation is, by definition,

$$
\delta^2 F_t(\mathbf{H}_t) \cdot \mathbf{V} := \frac{\mathrm{d}^2}{\mathrm{d}s^2}_{|s=0} F_t(\mathbf{H}_t + s\mathbf{V})
$$

where $\mathbf{V} \in W_0^{1,2}(\Omega, \mathbf{S}_0)$ is a fixed perturbation (see [71, 95] for similar computations on a 3D droplet). By inspecting Equation (3.3.9) and collecting all the quadratic terms in $\mathbf{V}$, it is straightforward to verify that the second variation is given by

$$
\begin{aligned}
\delta^2 F_t(\mathbf{H}_t) \cdot \mathbf{V} = & \int_\Omega \left\{ |\nabla \mathbf{V}|^2 + t\left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 + \frac{t}{2}|\mathbf{V}|^2 \left(h_t^2 - 1\right) \right\} \\
& + \lambda(t) \int_\Omega \left\{ 3\left(\mathbf{H}_t \cdot \mathbf{V}\right)^2 + \frac{3}{2} h_t^2 |\mathbf{V}|^2 + 3h_t |\mathbf{V}|^2 - 9h_t \left(\mathbf{n}_i \mathbf{V}_{ij}\right)^2 \right\}.
\end{aligned}
\tag{3.3.11}
$$

The second variation can be equivalently expressed in terms of v_0, v_1, v_2, v_3, v_4 in (3.3.10) as shown below:

$$
\begin{aligned}
\delta^2 F_t(\mathbf{H}_t) \cdot \mathbf{V} = & \int_\Omega \left\{ |\nabla \mathbf{V}|^2 + \frac{t}{2}|\mathbf{V}|^2 \left(h_t^2 - 1\right) + \frac{2t}{3} h_t^2 v_0^2 \right\} \\
& + \lambda(t) \int_\Omega \left\{ v_0^2 \left(3h_t^2 - 2h_t\right) + 3\left(h_t^2 + 2h\right)\left(v_3^2 + v_4^2\right) + 3\left(h_t^2 - h_t\right)\left(v_1^2 + v_2^2\right) \right\}.
\end{aligned}
\tag{3.3.12}
$$

Theorem 3.3.3. *The radial-hedgehog solution, $\mathbf{H}_t$, is a locally stable equilibrium of the Landau-de Gennes energy (3.2.3), in the space $\mathscr{A}$ i.e.*

$$
\delta^2 F_t(\mathbf{H}_t) \cdot \mathbf{V} > 0
$$

for all $t \geq 0$ and

$$
1 < R < \min\left\{ R^*, 1 + \frac{\pi}{\sqrt{6}} \right\},
$$

where R^* has been defined in Proposition 3.3.1.

Proof. The proof follows from a Hardy-type trick. We start with the integral expression (3.3.12). We recall from Proposition 3.3.2 that for $R < R^*$, we have

$$
\frac{2}{3} \leq h_t(r) \leq 1 \quad \text{for any } 1 \leq r \leq R
$$

so that $3h_t^2 - 2h_t \geq 0$ for $r \in [1, R]$. Therefore, there are two problematic non-positive terms above in (3.3.12): $|\mathbf{V}|^2\left(h_t^2 - 1\right)$ and $\left(h_t^2 - h_t\right)\left(v_1^2 + v_2^2\right)$. We combine the two non-positive terms as shown below:

$$
\begin{aligned}
\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} = &\int_\Omega \left\{ |\nabla\mathbf{V}|^2 + |\mathbf{V}|^2\left(\frac{t}{2}\left(h_t^2 - 1\right) + \frac{3\lambda(t)}{2}\left(h_t^2 - h_t\right)\right)\right\} \\
&+ \frac{2t}{3}\int_\Omega h_t^2 v_0^2 + \lambda(t)\int_\Omega \left\{ \left(3h_t^2 - 2h_t\right)v_0^2 + 3\left(h_t^2 + 2h\right)\left(v_3^2 + v_4^2\right)\right\} \\
&+ \frac{3\lambda(t)}{2}\int_\Omega \left(h_t - h_t^2\right)\left(\frac{2}{3}v_0^2 + 2v_3^2 + 2v_4^2\right).
\end{aligned}
$$

The second variation is bounded from below by

$$
\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} \geq \int_\Omega \left\{ |\nabla\mathbf{V}|^2 + |\mathbf{V}|^2\left(\frac{t}{2}(h_t^2 - 1) + \frac{3\lambda(t)}{2}\left(h_t^2 - h_t\right)\right)\right\}. \tag{3.3.13}
$$

An arbitrary $\mathbf{V}$ can be written as

$$
\mathbf{V}(x) = h_t(r)\bar{\mathbf{V}}(x)
$$

where $\bar{\mathbf{V}}$ vanishes on $r = 1$ and $r = R$, since h_t is strictly positive for $1 < r < R$. Therefore,

$$
|\nabla\mathbf{V}|^2 = \left(\frac{\mathrm{d}h_t}{\mathrm{d}r}\right)^2 |\bar{\mathbf{V}}|^2 + h_t^2(r)|\nabla\bar{\mathbf{V}}|^2 + 2h_t(r)\frac{\mathrm{d}h_t}{\mathrm{d}r}\frac{x_k}{r}\bar{\mathbf{V}}_{ij}\bar{\mathbf{V}}_{ij,k}. \tag{3.3.14}
$$

We use integration by parts to compute

$$
\begin{aligned}
\int_\Omega h_t(r)\frac{\mathrm{d}h_t}{\mathrm{d}r}\frac{x_k}{r}\bar{\mathbf{V}}_{ij}\bar{\mathbf{V}}_{ij,k} = &\int_\Omega \frac{\partial}{\partial x_k}\left(h_t\frac{\mathrm{d}h_t}{\mathrm{d}r}|\bar{\mathbf{V}}|^2\frac{x_k}{r}\right) \\
&- \int_\Omega |\bar{\mathbf{V}}|^2\left(\left(\frac{\mathrm{d}h_t}{\mathrm{d}r}\right)^2 + h_t\frac{\mathrm{d}^2 h_t}{\mathrm{d}r^2} + 2\frac{h_t}{r}\frac{\mathrm{d}h_t}{\mathrm{d}r}\right).
\end{aligned}
$$

Since $\bar{\mathbf{V}}$ vanishes on $\partial\Omega$, the boundary contribution vanishes too. Thus, we obtain

$$
\int_\Omega |\nabla\mathbf{V}|^2 = \int_0^{2\pi}\int_0^{\pi}\int_1^R \left(h_t^2 r^2|\nabla\bar{\mathbf{V}}|^2 - |\bar{\mathbf{V}}|^2 h_t\frac{\mathrm{d}^2 h_t}{\mathrm{d}r^2}r^2 - 2h_t\frac{\mathrm{d}h_t}{\mathrm{d}r}r|\bar{\mathbf{V}}|^2\right)\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi. \tag{3.3.15}
$$

Recalling the ordinary differential equation for the function $h_t(r)$ in (3.3.4), we see that

$$
\begin{aligned}
&\int_\Omega \left(\frac{t}{2}(h_t^2 - 1) + \frac{3\lambda(t)}{2}\left(h_t^2 - h_t\right)\right)|\mathbf{V}|^2 = \\
&\qquad \int_0^{2\pi}\int_0^{\pi}\int_1^R \left(\frac{\mathrm{d}^2 h_t}{\mathrm{d}r^2} + \frac{2}{r}\frac{\mathrm{d}h_t}{\mathrm{d}r} - 6\frac{h_t}{r^2}\right)h_t|\bar{\mathbf{V}}|^2 r^2\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi.
\end{aligned} \tag{3.3.16}
$$

Combining (3.3.13), (3.3.15) and (3.3.16), we obtain

$$
\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} \geq \int_0^{2\pi}\int_0^{\pi}\int_1^R h_t^2(r)\left(r^2|\nabla\bar{\mathbf{V}}|^2 - 6|\bar{\mathbf{V}}|^2\right)\sin\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi. \tag{3.3.17}
$$

We now use $r \geq 1$ and Wirtinger's inequality [46]

$$
\int_1^R \left(\frac{\partial v}{\partial r}\right)^2 \mathrm{d}r \geq \frac{\pi^2}{(R-1)^2}\int_1^R v^2\,\mathrm{d}r
$$

for any function $v\colon [1, R] \to \mathbb{R}$ such that $v(1) = v(R) = 0$, to obtain $\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} > 0$ for

$$
(R-1)^2 < \frac{\pi^2}{6}.
$$

□

3.4 On the minimality of the hedgehog when $R-1$ is small

This section is devoted to the proof of Theorem 3.1.1, i.e., we assume that $R-1$ is small and prove that the radial-hedgehog is energy minimizing. As a preliminary remark, we point out that the smallness assumption (3.1.1) on $R-1$ and Proposition 3.3.1 imply

$$h_t(r) \geq \frac{2}{3} \quad \text{for} \quad 1 \leq r \leq R. \tag{3.4.1}$$

Take an admissible field $\mathbf{Q} \in \mathscr{A}$ and set $\mathbf{V} := \mathbf{Q} - \mathbf{H}_t \in W_0^{1,2}(\Omega, \mathbf{S}_0)$. The functions $v_0, v_1, \ldots, v_4$, are the coordinates of $\mathbf{V}$ with respect to the basis $\mathbf{E}$, $\mathbf{F}$, $\mathbf{G}$, $\mathbf{X}$, $\mathbf{Y}$:

$$\mathbf{V} = v_0\mathbf{E} + v_1\mathbf{F} + v_2\mathbf{G} + v_3\mathbf{X} + v_4\mathbf{Y}.$$

We have an expression for the energy difference $F_t(\mathbf{Q}) - F_t(\mathbf{H}_t)$, namely, Equation (3.3.9):

$$\begin{aligned} F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) = \int_\Omega \Big\{ & \frac{1}{2}\left|\nabla\mathbf{V}\right|^2 + \frac{t}{4}\left|\mathbf{V}\right|^2(h_t^2 - 1) + \frac{t}{2}(\mathbf{H}_t\cdot\mathbf{V})^2 \\ & + \frac{\lambda(t)}{8}\left(6h^2\left|\mathbf{V}\right|^2 + 12(\mathbf{H}_t\cdot\mathbf{V})^2 - 12\sqrt{6}\,\mathrm{tr}\left(\mathbf{H}_t\mathbf{V}^2\right)\right) \\ & + \frac{t}{2}(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 + \frac{\lambda(t)}{8}\left(12(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 - 4\sqrt{6}\,\mathrm{tr}\,\mathbf{V}^3\right) \\ & + \frac{t}{8}\left|\mathbf{V}\right|^4 + \frac{3\lambda(t)}{8}\left|\mathbf{V}\right|^4 \Big\}. \end{aligned}$$

A direct computation shows that

$$-12\sqrt{6}\left(\mathbf{H}_t\mathbf{V}^2\right) = -4h\left(v_0^2 - 9v_3^2 - 9v_4^2\right) - 6h\left|\mathbf{V}\right|^2,$$

so

$$\begin{aligned} F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) = \int_\Omega \Big\{ & \frac{1}{2}\left|\nabla\mathbf{V}\right|^2 + \frac{t}{4}\left|\mathbf{V}\right|^2(h_t^2 - 1) + \frac{t}{2}(\mathbf{H}_t\cdot\mathbf{V})^2 \\ & + \frac{3\lambda(t)}{4}\left|\mathbf{V}\right|^2(h_t^2 - h_t) + \frac{\lambda(t)}{8}\left(12(\mathbf{H}_t\cdot\mathbf{V})^2 - 4h\left(v_0^2 - 9v_3^2 - 9v_4^2\right)\right) \\ & + \frac{t}{2}(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 + \frac{\lambda(t)}{8}\left(12(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 - 4\sqrt{6}\,\mathrm{tr}\,\mathbf{V}^3\right) \\ & + \frac{t}{8}\left|\mathbf{V}\right|^4 + \frac{3\lambda(t)}{8}\left|\mathbf{V}\right|^4 \Big\} \\ = \int_\Omega \Big\{ & \frac{1}{2}\left|\nabla\mathbf{V}\right|^2 + \frac{1}{2}f(h_t)\left|\mathbf{V}\right|^2 + \lambda(t)\left(-\frac{\sqrt{6}}{2}\,\mathrm{tr}\,\mathbf{V}^3 + \frac{h}{2}\left(-v_0^2 + 9v_3^2 + 9v_4^2\right)\right) \\ & + \frac{t + 3\lambda(t)}{8}\left(2(\mathbf{H}_t\cdot\mathbf{V}) + \left|\mathbf{V}\right|^2\right)^2 \Big\}, \end{aligned} \tag{3.4.2}$$

where $f(h) := \frac{t}{2}(h^2 - 1) + \frac{3\lambda(t)}{2}\left(h^2 - h\right)$. To deal with the first two terms, we write $\mathbf{V} = h_t\mathbf{W}$, $v_i = h_t w_i$ and use the Hardy decomposition trick again. With computations similar to (3.3.14)–(3.3.17), we obtain

$$\begin{aligned} F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) = \int_\Omega \Big\{ & h_t^2\left(\frac{1}{2}\left|\nabla\mathbf{W}\right|^2 - \frac{3}{r^2}\left|\mathbf{W}\right|^2\right) + \lambda(t)\,h_t^3\,\psi(\mathbf{W}) \\ & + \frac{t + 3\lambda(t)}{8}h_t^4\left(2\left(\frac{\mathbf{H}_t}{h_t}\cdot\mathbf{W}\right) + \left|\mathbf{W}\right|^2\right)^2 \Big\} \end{aligned} \tag{3.4.3}$$

where

$$
\begin{aligned}
\psi(\mathbf{W}) &:= -\frac{\sqrt{6}}{2}\operatorname{tr}\mathbf{W}^3 - \frac{1}{2}w_0^2 + \frac{9}{2}w_3^2 + \frac{9}{2}w_4^2 \\
&= -\frac{1}{2}w_0^2 + \frac{9}{2}\left(w_3^2 + w_4^2\right) + \sqrt{6}w_0\left(w_3^2 + w_4^2\right) \\
&\quad + \frac{3\sqrt{6}}{2}w_4\left(w_2^2 - w_1^2\right) - 3\sqrt{6}w_1w_2w_3 - \frac{\sqrt{6}}{2}w_0\left(w_1^2 + w_2^2\right) - \frac{\sqrt{6}}{9}w_0^3.
\end{aligned}
\tag{3.4.4}
$$

In order to prove Theorem 3.1.1, we need to show $F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq 0$ for any admissible $\mathbf{Q}$, with equality if and only if $\mathbf{Q} = \mathbf{H}_t$. In the following lemmas, we prove that the global contribution of the $\lambda(t)$-dependent terms in (3.4.3) is non-negative, provided that (3.4.1) holds. Since $R-1$ is assumed to be small, the gradient-squared term compensates for the negative term $-3|\mathbf{W}|^2/r^2$. This completes the proof of the theorem.

Lemma 3.4.1. *Let ψ be defined by Formula* (3.4.4)*, we have*

$$
\psi(w_0,\, w_1,\, w_2,\; w_3,\, w_4) \geq \psi\left(w_0,\, \sqrt{w_1^2 + w_2^2},\, 0,\, 0,\, \sqrt{w_3^2 + w_4^3}\right).
$$

for all $(w_0,\, w_1,\, w_2,\, w_3,\, w_4) \in \mathbb{R}^5$.

Proof. Thanks to (3.4.4), the lemma boils down to proving

$$
\frac{3\sqrt{6}}{2}w_4\left(w_2^2 - w_1^2\right) - 3\sqrt{6}w_1w_2w_3 \geq -\frac{3\sqrt{6}}{2}\sqrt{w_3^2 + w_4^2}\left(w_1^2 + w_2^2\right).
\tag{3.4.5}
$$

Let us consider the change of variables given by

$$
w_1 = \rho\cos\theta\cos\varphi_1, \qquad w_2 = \rho\cos\theta\sin\varphi_1, \qquad w_3 = \rho\sin\theta\cos\varphi_2, \qquad w_4 = \rho\sin\theta\sin\varphi_2,
$$

where

$$
\rho > 0, \qquad 0 \leq \theta \leq \frac{\pi}{2}, \qquad 0 \leq \varphi_1, \varphi_2 < 2\pi.
$$

This formula defines an admissible change of variable, because $(\rho,\, \theta,\, \varphi_1,\, \varphi_2) \mapsto (w_1,\, w_2,\, w_3,\, w_4)$ gives a one-to-one and onto mapping $(0, +\infty) \times [0, \pi/2] \times [0, 2\pi)^2 \to \mathbb{R}^4 \setminus \{0\}$. We write the left-hand side of (3.4.5) in terms of the new variables and obtain

$$
\begin{aligned}
&\frac{3\sqrt{6}}{2}w_4\left(w_2^2 - w_1^2\right) - 3\sqrt{6}w_1w_2w_3 \\
&\qquad = \frac{3\sqrt{6}}{2}\rho^3\sin\theta\cos^2\theta\left(\left(\sin^2\varphi_1 - \cos^2\varphi_1\right)\sin\varphi_2 - 2\sin\varphi_1\cos\varphi_1\cos\varphi_2\right) \\
&\qquad = -\frac{3\sqrt{6}}{2}\rho^3\sin\theta\cos^2\theta\left(\cos(2\varphi_1)\sin\varphi_2 + \sin(2\varphi_1)\cos\varphi_2\right) \\
&\qquad = -\frac{3\sqrt{6}}{2}\rho^3\sin\theta\cos^2\theta\sin\left(2\varphi_1 + \varphi_2\right) \\
&\qquad \geq -\frac{3\sqrt{6}}{2}\rho^3\sin\theta\cos^2\theta,
\end{aligned}
$$

which is precisely the right-hand side of (3.4.5). □

Lemma 3.4.2. *If* (3.4.1) *holds, then*

$$
\psi(\mathbf{W}) + \frac{3h}{8}\left(2\frac{\mathbf{H}_t}{h_t}\cdot\mathbf{W} + |\mathbf{W}|^2\right)^2 \geq 0.
$$

Proof. It is convenient to express the function ψ in terms of a new set of variables for the proof of this lemma. Throughout the proof, we assume without loss of generality that $w_2 = w_3 = 0$ (see Lemma 3.4.1). Let

$$X := \sqrt{\frac{2}{3}}(w_0 + 3w_4) \tag{3.4.6}$$

and

$$\epsilon := 2\frac{\mathbf{H}_t}{h_t} \cdot \mathbf{W} + |\mathbf{W}|^2 = \frac{2}{3}w_0^2 + 2\sqrt{\frac{2}{3}}w_0 + 2w_1^2 + 2w_4^2. \tag{3.4.7}$$

Substituting

$$w_1^2 = \frac{\epsilon}{2} - \frac{1}{3}w_0^2 - \sqrt{\frac{2}{3}}w_0 - w_4^2$$

and

$$w_0 = \sqrt{\frac{3}{2}}X - 3w_4$$

into the right-hand side of (3.4.4), we obtain

$$\psi(\mathbf{W}) = \frac{1}{4}\left(X^3 + 3X^2 - 3\epsilon X\right). \tag{3.4.8}$$

Thus, ψ reduces to a polynomial of degree three in the variables X and ϵ.

Our goal is to minimize ψ and we need to demarcate the relevant ranges for the variables X and ϵ. Firstly, we deduce that (see Equation (3.4.7))

$$\epsilon = \left|\frac{\mathbf{H}_t}{h_t} + \mathbf{W}\right|^2 - 1 = \left|\frac{\mathbf{Q}}{h_t}\right|^2 - 1 \geq -1.$$

Then (3.4.7) implies that

$$\frac{2}{3}w_0^2 + 2\sqrt{\frac{2}{3}}w_0 + 2w_4^2 \leq \epsilon. \tag{3.4.9}$$

This inequality can be written in the equivalent form

$$\frac{2}{3}\left(w_0 + \sqrt{\frac{3}{2}}\right)^2 + 2w_4^2 \leq 1 + \epsilon,$$

from which it is clear that (3.4.9) represents a region bounded by an ellipse in the $(w_0,\, w_4)$-plane. We denote that region by Σ. Then, X can take any value between the minimum and the maximum of the function $F\colon (w_0,\, w_4) \mapsto \sqrt{2/3}(w_0 + 3w_4)$ over Σ. By the Lagrange multiplier theorem, at the extrema the tangent lines to the ellipse $\partial\Sigma$ have equation $\sqrt{2/3}(w_0 + 3w_4) = c$. Thus, the minimum and the maximum value of F over Σ are exactly the values of c for which the line $\sqrt{2/3}(w_0 + 3w_4) = c$ is tangent to $\partial\Sigma$. These values can be computed, e.g., by forcing the system for $(w_0,\, w_4)$

$$\frac{2}{3}w_0^2 + 2\sqrt{\frac{2}{3}}w_0 + 2w_4^2 = \epsilon, \qquad \sqrt{\frac{2}{3}}(w_0 + 3w_4) = c$$

to have a unique solution. Through some simple algebra, one concludes that

$$-1 - 2\sqrt{\epsilon + 1} \leq X \leq -1 + 2\sqrt{\epsilon + 1}. \tag{3.4.10}$$

Next, we minimize the right-hand side of (3.4.8), as a function of X, in the range (3.4.10). We obtain

$$\psi(\mathbf{W}) \geq \psi\left(-1 + \sqrt{\epsilon + 1}\right) = \frac{3}{4}\epsilon + \frac{1}{2} - \frac{1}{2}(\epsilon + 1)^{3/2},$$

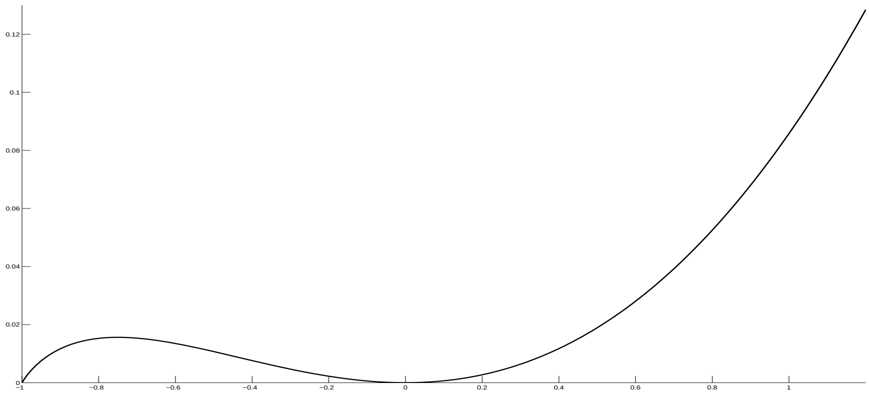

Figure 3.1: A plot of of the function G.

hence, if the condition (3.4.1) is satisfied and $h_t \geq \frac{2}{3}$,

$$\psi(\mathbf{W}) + \frac{3h}{8}\left(2\frac{\mathbf{H}_t}{h_t}\cdot\mathbf{W} + |\mathbf{W}|^2\right)^2 \geq \frac{1}{4}\epsilon^2 + \frac{3}{4}\epsilon + \frac{1}{2} - \frac{1}{2}(\epsilon+1)^{3/2} =: G(\epsilon).$$

Finally, we need to show that the function G is non negative on $[-1, +\infty)$. An easy analysis shows that G has a global minimum on $[-1, +\infty)$, which is either $\epsilon = -1$ or an interior critical point. Now, $G(-1) = 0$, and there are two critical points for G: $\epsilon = -3/4$ (which is a local maximum) and $\epsilon = 0$. Therefore, $G(\epsilon) \geq 0$ for every $\epsilon \geq -1$. ☐

Lemma 3.4.3. *For all $R > 1$ there exists a (optimal) constant $C_H(R) > 0$ such that, for all $v \in H^1_0(1, R)$, we have*

$$\int_1^R v'^2 r^2 \,\mathrm{d}r \geq C_H(R) \int_1^R v^2 \,\mathrm{d}r.$$

Moreover, $C_H(R) > 1/4$ for all $R > 1$.

Proof. We consider the following minimization problem with constraints:

$$C_H(R) := \min\left\{\int_1^R r^2 v'^2 \,\mathrm{d}r \colon v \in H^1_0(1, R), \int_1^R v^2 \,\mathrm{d}r = 1\right\}.$$

Using standard methods in the calculus of variations, one can easily see that a minimizer exists. By Lagrange's multiplier theorem, any minimizer solves the eigenvalue problem

$$\begin{cases} -\dfrac{\mathrm{d}}{\mathrm{d}r}\left(r^2 v'(r)\right) = \lambda v(r) \\ v(1) = v(R) = 0, \end{cases} \tag{3.4.11}$$

and, in particular,

$$r^2 v'' + 2rv' + \lambda r = 0.$$

This equation can be easily solved, e.g., with the change of variable $r = e^t$, $u(t) = v(r)$. One finds a necessary and sufficient condition for the existence of a non-trivial solution $v \not\equiv 0$ to (3.4.11), namely that

$$\lambda = \lambda_k(R) := \frac{k^2\pi^2}{\log R} + \frac{1}{4} \qquad \text{for some } k \in \mathbb{N} \setminus \{0\}.$$

Thus, the λ_k's are the eigenvalues for (3.4.11) and

$$C_H(R) = \lambda_1(R) = \frac{\pi^2}{\log R} + \frac{1}{4}. \tag{3.4.12}$$

This proves the lemma. □

The proof of Theorem 3.1.1 now readily follows from the previous lemmas.

Proof of Theorem 3.1.1. To prove the minimality of the hedgehog, we must show that

$$F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq 0.$$

By Equation (3.4.3), we have

$$F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq \int_\Omega h_t^2 \left(\frac{1}{2} |\nabla \mathbf{W}|^2 - \frac{3}{r^2} |\mathbf{W}|^2 \right) + \int_\Omega \lambda(t) h_t^3 \left\{ \psi(\mathbf{W}) + \frac{3h}{8} \left(2\frac{\mathbf{H}_t}{h_t} \cdot \mathbf{W} + |\mathbf{W}|^2 \right)^2 \right\}.$$

By virtue of (3.4.1) and Lemma 3.4.2, the second integral is non negative and we obtain

$$F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq \int_\Omega \frac{4}{9} \left(\frac{1}{2} |\nabla \mathbf{W}|^2 - \frac{3}{r^2} |\mathbf{W}|^2 \right).$$

If we write the integral using spherical coordinates, apply Fubini's theorem and Lemma 3.4.3, we get

$$F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq \frac{4}{9} \left(\frac{1}{2} C_H(R) - 3 \right) \int_\Omega \frac{1}{r^2} |\mathbf{W}|^2.$$

The constant $C_H(R)$ is given explicitly by (3.4.12). Finally, we recall the assumption (3.1.1) which yields

$$\frac{1}{2} C_H(R) - 3 = \frac{\pi^2}{2 \log R} - \frac{23}{8} > 0.$$

Hence, we conclude that $F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq 0$, with equality if and only if $\mathbf{Q} = \mathbf{H}_t$. □

3.5 Minimality of the hedgehog for large t

This section is devoted to the proof of Theorem 3.1.2, i.e., showing that the radial-hedgehog is energy-minimizing for all $R > 1$ and large t. As a preliminary step, we adapt the proof by Ignat et al. [73] and prove that the radial-hedgehog is locally stable (i.e., the second variation of the energy is positive) when the temperature t is large enough, without restriction on $R - 1$. We first show that the temperature t uniformly controls the magnitude of the radial-hedgehog solution, for large enough $t > 0$.

Lemma 3.5.1. *Let $h_t \in H^1(1, R)$ be a minimizer of*

$$E(h) := \int_1^R \left\{ \frac{1}{2} h'^2 + \frac{3}{r^2} h^2 + \frac{t}{8} (1 - h^2)^2 + \frac{\lambda(t)}{8} (1 + 3h^4 - 4h^3) \right\} r^2 \mathrm{d}r, \tag{3.5.1}$$

with the boundary conditions $h_t(1) = h_t(R) = 1$. Then, $0 < h_t \leq 1$ for all $t \geq 0$. Moreover,

$$h_t \to 1 \qquad \textit{uniformly as } t \to \infty.$$

Proof. The bounds $0 < h_t \leq 1$ are easily established [95, 96]. Indeed, $h_t \geq 0$ from the energy minimality of h_t (refer to (3.5.1)). The function $h_t \leq 1$, as an immediate consequence of the maximum principle. We can easily prove that $h_t > 0$. Indeed, we assume that there exists a point r_1 such that $h_t(r_1) = 0$. Since we know that $h_t \geq 0$, r_1 must be a minimum point for h_t, so $h_t'(r_1) = 0$. Then we apply the classical well-posedness theory for Cauchy problems for ODE's and conclude that $h_t \equiv 0$, which contradicts the boundary conditions $h_t(1) = h_t(R) = 1$. Thus, we must have $h_t > 0$.

Finally, we check the uniform convergence of h_t as $t \to \infty$. Let $r_{\min} \in (1, R)$ be a minimum point for h_t. We have $h_t''(r_{\min}) \geq 0$ and $h_t'(r_{\min}) = 0$. Therefore, by Equation (3.3.4),

$$-\frac{6}{r_{\min}^2} h_t(r_{\min}) \leq f(h_t(r_{\min}))h_t(r_{\min}) \leq \frac{t}{2}\left(h_t^2(r_{\min}) - 1\right) h_t(r_{\min}).$$

We divide by $h_t(r_{\min}) > 0$ and obtain

$$1 - h_t^2(r_{\min}) \leq \frac{12}{t r_{\min}^2} \leq \frac{12}{t}.$$

Thus,

$$1 \geq h_t \geq \sqrt{1 - \frac{12}{t}} \to 1 \qquad \text{as } t \to +\infty, \text{ uniformly on } (1, R). \qquad \square$$

The second step in our analysis for large t is the study of the second variation of the energy. Recall that, given a variation $\mathbf{V} \in W_0^{1,2}(\Omega, \mathbf{S}_0)$ (i.e., $\mathbf{Q} = \mathbf{H}_t + \mathbf{V}$), the second variation is given by

$$\frac{1}{2}\delta^2 F_t(\mathbf{H}_t) \cdot \mathbf{V} = \int_\Omega \left\{ \frac{1}{2}\left|\nabla \mathbf{V}\right|^2 + \frac{1}{3} f_0(h_t) v_0^2 + f_2(h_t)(v_1^2 + v_2^2) + f_4(h_t)(v_3^2 + v_4^2) \right\} \tag{3.5.2}$$

(see Equation (3.3.11)), where $v_0, \ldots, v_4$ are the coordinates of $\mathbf{V}$ with respect to the basis we have chosen and

$$\begin{aligned} f_0(h) &:= \frac{t}{2}\left(3h^2 - 1\right) + \frac{3\lambda(t)}{2}\left(3h^2 - 2h\right) \\ f_2(h) &:= \frac{t}{2}\left(h^2 - 1\right) + \frac{3\lambda(t)}{2}\left(h^2 - h\right) \\ f_4(h) &:= \frac{t}{2}\left(h^2 - 1\right) + \frac{3\lambda(t)}{2}\left(h^2 + 2h\right). \end{aligned} \tag{3.5.3}$$

We want to show that the second variation is positive for every choice of $\mathbf{V}$ and large enough t. In [73], it is shown that the analysis of $\delta^2 F_t(\mathbf{H}_t)$ can be reduced to the study of the simpler functionals $\phi_{0,i}$, defined for $i \in \mathbb{N}$ by

$$\begin{aligned} \phi_{0,0}(v_0) &:= \frac{2}{3}\int_1^R \left\{ |v_0'|^2 + \frac{6}{r^2} v_0^2 + f_0(h_t) v_0^2 \right\} r^2 \, \mathrm{d}r, \\ \phi_{0,i}(v_0,\, v_2,\, v_4) &:= \int_1^R \left\{ \frac{\lambda_{0,i}}{3} |v_0'|^2 + |v_2'|^2 + (\lambda_{0,i} - 2)|v_4'|^2 \right. \\ &\qquad + \frac{1}{r^2}\left(\frac{\lambda_{0,i}(\lambda_{0,i} + 6)}{3} v_0^2 + (\lambda_{0,i} + 4) v_2^2 + (\lambda_{0,i} - 2)^2 v_4^2 \right. \\ &\qquad\qquad \left. - 4\lambda_{0,i}\, v_0\, v_2 + 4(\lambda_{0,i} - 2)\, v_2\, v_4 \right) \\ &\qquad \left. + \frac{\lambda_{0,i}}{3} f_0(h_t) v_0^2 + f_2(h_t) v_2^2 + (\lambda_{0,i} - 2) f_4(h_t) v_4^2 \right\} r^2 \, \mathrm{d}r. \end{aligned} \tag{3.5.4}$$

The functions v_0, v_2 and v_4 depend on the radial variable r alone and belong to

$$H_0^1(1,\, R) = \left\{ w \in L^2([1,\, R],\, \mathrm{d}r) \colon w' \in L^2([1,\, R],\, r^2 \mathrm{d}r),\, w(1) = w(R) = 0 \right\},$$

and $\lambda_{0,i} := i(i+1)$. More precisely, combining [73, Proposition 3.2] and [73, Proposition 3.4.(b)], we see that $\frac{1}{2}\delta^2 F_t(\mathbf{H}_t)$ can be written as a linear combination, with positive weights, of the $\phi_{0,i}$'s. Thus, if the $\phi_{0,i}$'s are non-negative (resp., positive definite) then $\delta^2 F_t(\mathbf{H}_t)$ is non-negative (resp., positive definite).

Arguing as in [73, Proposition 4.1, Lemma 4.2], we can show that $\phi_{0,i} \geq 0$ for $i \geq 4$ and that $\phi_{0,3} \geq 0$ if $\phi_{0,2} \geq 0$. Note that the functions f_0, f_2, f_4 which are considered in [73] are *not* given by (3.5.3). However, all the results we are appealing to are independent of the specific form of f_0, f_2, f_4; they only rely on manipulations of the gradient terms, which are the same. Therefore, we just need to study the functionals $\phi_{0,i}$ for $i \in \{0,\, 1,\, 2\}$. To this purpose, we cannot use the same method as in [73], because in our case h_t has an intermediate minimum in $[0,\, 1]$ and h_t' is not positive everywhere. Instead, we use the Hardy decomposition trick, i.e. we write the variables v_i as $v_i = hw_i$, where h_t is the hedgehog profile and is a classical solution of the differential equation (3.3.4).

Lemma 3.5.2. *Consider the functional*

$$\phi(v) := \int_1^R \left\{ \alpha {v'}^2 + \frac{\beta}{r^2} v^2 + \alpha \left(f(h_t) + \gamma \right) v^2 \right\} r^2 \,\mathrm{d}r, \tag{3.5.5}$$

defined for $v \in H^1_0(1,\, R)$, where $f = f_2$ is given by (3.5.3)*, h_t is a minimizer of* (3.5.1)*, and α, β, $\gamma \in \mathbb{R}$ are fixed parameters. Then ϕ can be equivalently written as*

$$\phi(v) = \int_1^R \left\{ \alpha \left(\frac{v}{h_t} \right)'^2 h_t^2 + \frac{\beta - 6\alpha}{r^2} v^2 + \alpha\gamma v^2 \right\} r^2 \,\mathrm{d}r.$$

Proof. Without loss of generality, we can assume that $v \in C^\infty_c(1,\, R)$ (the general case is recovered by a density argument). Since $h_t > 0$, we can write $v = h_t w$, with $w \in C^\infty_c(1,\, R)$. By substitution in (3.5.5), and using Equation (3.3.4), we have

$$\begin{aligned} \phi(v) &= \int_1^R \left\{ \alpha (h_t' w + h_t w')^2 + \frac{\beta}{r^2} h_t^2 w^2 + \alpha \left(h_t'' + \frac{2}{r} h_t' - \frac{6}{r^2} h_t \right) h_t w^2 + \alpha\gamma h_t^2 w^2 \right\} r^2 \,\mathrm{d}r \\ &= \int_1^R \left\{ \alpha {w'}^2 + \frac{\beta}{r^2} w^2 - \frac{6\alpha}{r^2} w^2 + \alpha\gamma w^2 \right\} h_t^2 r^2 \,\mathrm{d}r \\ &\quad + \int_1^R \left\{ \alpha {h_t'}^2 w^2 + 2\alpha h_t h_t' w w' + \alpha h_t h_t'' w^2 + \frac{2\alpha}{r} h_t h_t' w^2 \right\} r^2 \,\mathrm{d}r. \end{aligned} \tag{3.5.6}$$

By an integration by parts, we see that

$$\alpha \int_1^R h_t h_t'' w^2 r^2 \,\mathrm{d}r = -\alpha \int_1^R \left\{ 2 h_t h_t' w w' r^2 + {h_t'}^2 w^2 r^2 + 2 h_t h_t' w^2 r \right\} \,\mathrm{d}r,$$

so the last integral in (3.5.6) vanishes, and the proof is complete. □

With the help of the previous lemma, we can now complete the analysis of the second variation.

Proposition 3.5.3. *There exists $t_* > 0$ such that the radial-hedgehog is a locally stable equilibrium for Problem* (LG_t)*, for all $t \geq t_*$ and $R > 1$.*

Proof. By the previous discussion, it is enough to prove the positivity of $\phi_{0,i}$ defined above, for $i \in \{0,\, 1,\, 2\}$. Throughout the proof, we fix v_0, v_2, $v_4 \in C^\infty_c(1,\, R)$, and set $w_k := v_k/h_t$ for $k \in \{0,\, 2,\, 4\}$. It is not restrictive to assume that the v_k's are regular, because $C^\infty_c(1,\, R)$ is dense in $H^1_0(1,\, R)$.

Step 0 (Study of $\phi_{0,0}$). We remark that in view of (3.5.3), we have

$$f_0(h_t) = f(h_t) + t h_t^2 + \frac{3\lambda(t)}{2} \left(2h_t^2 - h_t \right). \tag{3.5.7}$$

Hence, we can apply Lemma 3.5.2 to $\phi_{0,0}$:

$$\frac{3}{2}\phi_{0,0}(v_0) = \int_1^R \left\{ |w_0'|^2 + \left(th_t^2 + \frac{3\lambda(t)}{2}(2h_t^2 - h_t) \right) w_0^2 \right\} h_t^2 r^2 \, \mathrm{d}r \, .$$

By Lemma 3.5.1, there exists $t_0 > 0$ such that $h_t \geq 1/2$ for $t \geq t_0$. As a consequence,

$$th_t^2 + \frac{3\lambda(t)}{2}(2h_t^2 - h_t) \geq \frac{1}{4}t_0 > 0$$

and $\phi_{0,0}(v_0) > 0$ when $t \geq t_0$, with equality if and only if $v_0 = 0$.

Step 1 (Study of $\phi_{0,1}$). We recall the definition of $\phi_{0,1}$, noting that $\lambda_{0,1} = 2$:

$$\phi_{0,1}(v_0,\, v_2) := \int_1^R \left\{ \frac{2}{3}|v_0'|^2 + |v_2'|^2 + \frac{1}{r^2}\left(\frac{16}{3}v_0^2 + 6v_2^2 - 8\, v_0\, v_2 \right) + \frac{2}{3}f_0(h_t)v_0^2 + f_2(h_t)v_2^2 \right\} r^2 \, \mathrm{d}r.$$

With the help of (3.5.7), we apply Lemma 3.5.2 first to terms in v_0, followed by terms in v_2. We obtain

$$\phi_{0,1}(v_0,\, v_2) = \int_1^R \left\{ \frac{2}{3}|w_0'|^2 + |w_2'|^2 + \frac{1}{r^2}\left(\frac{4}{3}w_0^2 - 8\, w_0\, w_2 \right) + \frac{2}{3}\left(th_t^2 + \frac{3\lambda(t)}{2}(2h_t^2 - h_t) \right) w_0^2 \right\} h_t^2 r^2 \, \mathrm{d}r.$$

By virtue of Lemma 3.4.3, we have

$$\begin{aligned} \phi_{0,1}(v_0,\, v_2) \geq & \int_1^R \left\{ \frac{2}{3}|w_0'|^2 + \frac{2}{3}\left(th_t^2 + \frac{3\lambda(t)}{2}(2h_t^2 - h_t) \right) w_0^2 \right\} h_t^2 r^2 \mathrm{d}r \\ & + \int_1^R \left\{ \frac{4}{3}h_{\min}^2 w_0^2 - 8|w_0\, w_2| + \frac{1}{4}h_{\min}^2 w_2^2 \right\} \mathrm{d}r, \end{aligned}$$

where $h_{\min} := \min_{[1,\, R]} h_t > 0$. For $t \geq t_0$, we have $h_{\min}^2/4 \geq 1/16$ and

$$-8|w_0\, w_2| \geq -256 w_0^2 - \frac{1}{16}w_2^2 \geq -256 w_0^2 - \frac{1}{4}h_{\min}^2 w_2^2.$$

Since h_t converges uniformly to 1 (see Lemma 3.5.1), there exists some $t_1 \geq t_0$ such that, for all $t \geq t_1$ and $r \geq 1$,

$$\frac{2}{3}\left(th_t^2 + \frac{3\lambda(t)}{2}(2h_t^2 - h_t) \right) h_{\min}^2 r^2 + \frac{4}{3}h_{\min}^2 \geq 256.$$

We combine these inequalities to obtain $\phi_{0,1}(v_0,\, v_2) \geq 0$ for $t \geq t_1$ (with equality if and only if $v_0 = v_2 = 0$).

Step 2 (Study of $\phi_{0,2}$). Recall that $\phi_{0,2}$ is given by

$$\begin{aligned} \phi_{0,2}(v_0,\, v_2,\, v_4) := \int_1^R \Big\{ & 2|v_0'|^2 + |v_2'|^2 + 4|v_4'|^2 + \frac{1}{r^2}\left(24v_0^2 + 10v_2^2 + 16v_4^2 - 24v_0v_2 + 16v_2v_4 \right) \\ & + 2f_0(h_t)v_0^2 + f_2(h_t)v_2^2 + 4f_4(h_t)v_4^2 \Big\} r^2 \, \mathrm{d}r \end{aligned}$$

(set $\lambda_{0,2} = 6$ in Equation (3.5.4)). Given that

$$f_4(h_t) = f(h_t) + \frac{9\lambda(t)}{2}h_t \tag{3.5.8}$$

and $f_0(h_t)$ is given by (3.5.7), we can apply Lemma 3.5.2:

$$\begin{aligned} \phi_{0,2}(v_0,\, v_2,\, v_4) = \int_1^R \Big\{ & 2|w_0'|^2 + |w_2'|^2 + 4|w_4'|^2 + \frac{1}{r^2}\left(12w_0^2 + 4w_2^2 - 8w_4^2 - 24w_0w_2 + 16w_2w_4 \right) \\ & + \left(2th_t^2 + 3\lambda(t)(2h_t^2 - h_t) \right) w_0^2 + 18\lambda(t)h_t w_4^2 \Big\} h_t^2 r^2 \, \mathrm{d}r. \end{aligned}$$

Clearly, we have

$$\phi_{0,2}(v_0,\,v_2,\,v_4) \geq \int_1^R \Big\{ 2|w_0'|^2 + |w_2'|^2 + 4|w_4'|^2 + \big(12 + 2th_t^2 + 3\lambda(t)(2h_t^2 - h_t)\big)\, w_0^2 \\ + 4w_2^2 + (18\lambda(t)h_{\min} - 8)\, w_4^2 - 24w_0w_2 + 16w_2w_4 \Big\} h_t^2 \,\mathrm{d}r. \tag{3.5.9}$$

By applying the Cauchy-Schwarz inequality, we obtain the following inequality

$$-24w_0w_2 + 16w_2w_4 \geq -72w_0^2 - 4w_2^2 - 32w_4^2.$$

Recalling that $h_t \to 1$ uniformly (see Lemma 3.5.1), it is possible to find $t = t_2 \geq 0$ such that

$$12 + 2th_t^2 + 3\lambda(t)(2h_t^2 - h_t) \geq 72 \qquad \text{and} \qquad 18\lambda(t)h_{\min} - 8 \geq 32$$

for $t \geq t_2$. Hence, from (3.5.9), we conclude that

$$\phi_{0,2}(v_0,\,v_2,\,v_4) \geq 2\,\|w_0'\|^2_{L^2(1,\,R)} + \|w_2'\|^2_{L^2(1,\,R)} + 4\,\|w_4'\|^2_{L^2(1,\,R)}\,,$$

for any $t \geq t_2$. In particular, $\phi_{0,2}(v_0,\,v_2,\,v_4) \geq 0$ and equality holds if and only if $v_0 = v_2 = v_4 = 0$.

In the previous steps, we have shown that $\phi_{0,0}$, $\phi_{0,1}$ and $\phi_{0,2}$ are positive definite in their arguments for $t \geq t_* := \max\{t_0,\,t_1,\,t_2\}$. By the results presented in [73], this is enough to prove the proposition. ☐

The same method of proof applies to the following result, which yields an improved lower bound for the second variation.

Proposition 3.5.4. *Let α, β be two parameters such that $0 < \alpha < 1/2$, $0 < \beta < 9/2$. There exists a $t^* \geq 1$ (depending on α, β) such that the inequality*

$$\frac{1}{2}\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} \geq \int_\Omega \left\{ \frac{t}{3}h_t^2 v_0^2 + \alpha\lambda(t)v_0^2 + \beta\lambda(t)\left(v_3^2 + v_4^2\right)\right\}$$

holds for any $t \geq t^*$, $R > 1$ and any function $\mathbf{V} \in W_0^{1,2}(\Omega,\,\mathbf{S}_0)$. Here the v_i's denote the components of $\mathbf{V}$ with respect to the basis $\mathbf{E}$, $\mathbf{F}$, $\mathbf{G}$, $\mathbf{X}$, $\mathbf{Y}$.

Proof. Consider the quantity

$$\mathscr{F}(\mathbf{V}) := \frac{1}{2}\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} - \int_\Omega \left\{ \frac{t}{3}h_t^2 v_0^2 + \alpha\lambda(t)v_0^2 + \beta\lambda(t)\left(v_3^2 + v_4^2\right)\right\}.$$

Using formula (3.5.2) for the second variation, we obtain

$$\mathscr{F}(\mathbf{V}) = \int_\Omega \Big\{ \frac{1}{2}\left|\nabla\mathbf{V}\right|^2 + \frac{1}{3}\left(f_0(h_t) - th_t^2 - 3\alpha\lambda(t)\right) v_0^2 \\ + f_2(h_t)(v_1^2 + v_2^2) + \left(f_4(h_t) - \beta\lambda(t)\right)(v_3^2 + v_4^2)\Big\}.$$

By virtue of (3.5.7) and (3.5.8), we can write

$$f_0(h_t) - th_t^2 - 3\alpha\lambda(t) = f(h_t) + \frac{3\lambda(t)}{2}\left(2h_t^2 - h_t - 2\alpha\right) \tag{3.5.10}$$

and

$$f_4(h_t) - \beta\lambda(t) = f(h_t) + \lambda(t)\left(\frac{9h}{2} - \beta\right). \tag{3.5.11}$$

Recalling that $h_t \to 1$ uniformly by Lemma 3.5.1 and since we have fixed $\alpha < 1/2$, $\beta < 9/2$, we deduce that

$$\frac{3\lambda(t)}{2}\left(2h_t^2 - h_t - 2\alpha\right) \to +\infty, \qquad \lambda(t)\left(\frac{9h}{2} - \beta\right) \to +\infty \tag{3.5.12}$$

as $t \to +\infty$. We can now apply the same arguments as in Proposition 3.5.3 to the functional $\mathscr{F}$. The proof carries over almost word by word. Namely, at the end of each step 0–2, one uses the property (3.5.12) to absorb the negative contributions. We conclude that there exists $t^* \geq 1$ such that

$$\mathscr{F}(\mathbf{V}) \geq 0 \qquad \text{for all } \mathbf{V} \in W_0^{1,2}(\Omega,\, \mathbf{S}_0)$$

for $t \geq t^*$. □

The final ingredient in the proof of Theorem 3.1.2 is Lemma 3.5.5 below. This result controls the non-quadratic terms in the energy difference, $F_t(\mathbf{Q}) - F_t(\mathbf{H}_t)$ (see Equation (3.4.2)).

Lemma 3.5.5. *There exists $h_* \in (0,\, 1)$ such that if $h_t \geq h_*$ everywhere on $[1,\, R]$, then*

$$\varphi(\mathbf{V}) := \frac{2}{5}v_0^2 + v_3^2 + v_4^2 - \frac{\sqrt{6}}{2}\operatorname{tr}\mathbf{V}^3 + \frac{3}{8}|\mathbf{V}|^4 + 5\left(2(\mathbf{H}_t\cdot\mathbf{V}) + |\mathbf{V}|^2\right)^2 \geq 0$$

for every $\mathbf{V} \in \mathbf{S}_0$, with equality if and only if $\mathbf{V} = 0$.

Proof. From Lemma 3.4.1, we can assume without loss of generality that $v_2 = v_3 = 0$, so

$$\begin{aligned}\varphi(v_0,\, v_1,\, v_4) = \frac{2}{5}v_0^2 + v_4^2 + \sqrt{6}\left(v_0v_4^2 - \frac{3}{2}v_4v_1^2 - \frac{1}{2}v_0v_1^2 - \frac{1}{9}v_0^3\right)\\ + \frac{3}{8}\left(\frac{2}{3}v_0^2 + 2v_1^2 + 2v_4^2\right)^2 + 5\left(\frac{2}{3}v_0^2 + 2\sqrt{\frac{2}{3}}h_tv_0 + 2v_1^2 + 2v_4^2\right)^2.\end{aligned}$$

As a function of $(v_0,\, v_1,\, v_4) \in \mathbb{R}^3$, φ is smooth and bounded from below, since

$$\varphi(v_0,\, v_1,\, v_4) \geq \sqrt{6}\left(v_0v_4^2 - \frac{3}{2}v_4v_1^2 - \frac{1}{2}v_0v_1^2 - \frac{1}{9}v_0^3\right) + \frac{3}{8}\left(\frac{2}{3}v_0^2 + 2v_1^2 + 2v_4^2\right)^2 \to +\infty$$

as $|(v_0,\, v_1,\, v_4)| \to +\infty$. Thus, φ has a global minimum, which is also a critical point. We claim that $v_0 = v_1 = v_4 = 0$ is the unique critical point for φ, when h_t is sufficiently close to 1. This implies, in particular, that $v_0 = v_1 = v_4 = 0$ is a global minimum of φ and the lemma follows. For the sake of simplicity, we denote the triplet $(v_0,\, v_1,\, v_4)$ by $(x,\, y,\, z)$.

Step 1 (Any critical point satisfies $y = 0$). A critical point $(x,\, y,\, z)$ is a solution of the system $\nabla\varphi = 0$, that is,

$$\begin{aligned}\sqrt{6}\left(z^2 - \frac{y^2}{2} - \frac{x^2}{3}\right) + \frac{86}{9}\,x\left(x^2 + 3\,y^2 + 3\,z^2\right) + \left(\frac{4}{5} + \frac{80}{3}\,h_t^2\right)x\\ + \frac{40}{3}\sqrt{6}\,h_t\left(x^2 + y^2 + z^2\right) = 0\\ \frac{\sqrt{6}}{9}\,y\left(-27\,z - 9\,x + 129\sqrt{6}\,z^2 + 129\sqrt{6}\,y^2 + 43\sqrt{6}\,x^2 + 240\,h_tx\right) = 0\\ 2\sqrt{6}\,xz - \frac{3}{2}\sqrt{6}\,y^2 + \frac{86}{3}\,zx^2 + 86\,zy^2 + 86\,z^3 + 2\,z + \frac{80}{3}\sqrt{6}\,h_txz = 0.\end{aligned} \tag{3.5.13}$$

Let $y \neq 0$. Then,

$$y^2 = \frac{1}{129\sqrt{6}}\left(27\,z + 9\,x - 129\sqrt{6}\,z^2 - 43\sqrt{6}\,x^2 - 240\,h_tx\right). \tag{3.5.14}$$

We substitute this value of y^2 into Equation (3.5.13). Note that the xy^2-term in the first equation expands into several terms:

$$\frac{86}{3}xy^2 = \sqrt{6}\,xz + \frac{2}{\sqrt{6}}\,x^2 - \frac{86}{3}\,xz^2 - \frac{86}{9}\,x^3 - \frac{160}{3\sqrt{6}}\,h_t x^2.$$

Thus, the cubic x^3 and xz^2-terms cancel out when we inject this expression into (3.5.13). Similarly, the xz^2 and z^3-terms in the third equation cancel out because

$$\frac{86}{3}zy^2 = 3\sqrt{6}\,z^2 + \sqrt{6}\,xz - 86\,z^3 - \frac{86}{3}\,x^2 z - \frac{160}{\sqrt{6}}\,h_t xz.$$

So all the cubic terms in (3.5.13) disappear and we obtain

$$\begin{aligned} \frac{329}{430}\,x + \frac{80}{43}\,hx + \frac{80}{43}\,h_t^2 x - \frac{9}{86}\,z + \frac{120}{43}\,h_t z + \frac{\sqrt{6}}{6}\,x^2 + \sqrt{6}\,xz + \frac{3}{2}\sqrt{6}\,z^2 = 0 \\ -\frac{9}{86}\,x + \frac{120}{43}\,hx + \frac{145}{86}\,z + \frac{\sqrt{6}}{2}\,x^2 + 3\sqrt{6}\,xz + \frac{9}{2}\sqrt{6}\,z^2 = 0 \end{aligned}$$

This system can be further simplified by taking a linear combination of the two equations (we multiply the first equation by 3, the second by -1 and add the two equations). We obtain

$$\begin{gathered} 516\,x + 600\,hx + 1\,200\,h_t^2 x - 430\,z + 1\,800hz = 0 \\ -9\,x + 240\,h_t x + 145\,z + 43\sqrt{6}\,x^2 + 258\sqrt{6}\,xz + +387\sqrt{6}\,z^2 = 0. \end{gathered}$$

This is a system of second degree in $(x,\,z)$, so it can be easily solved. There are two solutions: $x = z = 0$, and $x = x_0(h_t)$, $z = z_0(h_t)$ where x_0, z_0 are algebraic functions of h_t. By substituting $x = x_0(h_t)$, $z = z_0(h_t)$ into Formula (3.5.14), we write y^2 as an algebraic function of h_t. Taking the limit as $h_t \to 1$, we get

$$y^2 \to -\frac{441\,133\,354\,650}{60\,505\,388\,947\,441} < 0$$

which is clearly a contradiction. Thus, there exists a value $h_0 \in (0,\,1)$ such that any critical point of φ satisfies $y = 0$ for $h_t \geq h_0$.

Step 2 (Any critical point satisfies $z = 0$). We set $y = 0$ in Equation (3.5.13):

$$\begin{aligned} \sqrt{6}\,z^2 - \frac{\sqrt{6}}{3}\,x^2 + \frac{86}{9}\,x\left(x^2 + 3\,z^2\right) + \left(\frac{4}{5} + \frac{80}{3}\,h_t^2\right)\,x + \frac{40}{3}\sqrt{6}\,h_t\left(x^2 + z^2\right) = 0 \\ \frac{\sqrt{6}}{9}\,z\left(3\sqrt{6} + 18\,x + 129\sqrt{6}\,z^2 + 43\sqrt{6}\,x^2 + 240\,h_t x\right) = 0 \end{aligned} \tag{3.5.15}$$

Suppose that $z \neq 0$. Then,

$$z^2 = -\frac{1}{129}\left(3 + 3\sqrt{6}\,x + 43\,x^2 + 40\sqrt{6}\,h_t x\right).$$

We eliminate the variable z from (3.5.15) and obtain an equation for x:

$$-860\sqrt{6}\,x^2 - 4\left(1 - 600\,h_t + 300\,h_t^2\right)\,x - 15\sqrt{6} - 200\sqrt{6}\,h_t = 0.$$

This equation has no real root for $h_t = 1$. Therefore, we conclude that there exists $h_* \in (h_0,\,1)$ such that any critical point of φ has $z = 0$ for $h_t \geq h_*$.

Step 3 (Conclusion). Substituting $y = z = 0$ into Equation (3.5.13) results in an equation for x:

$$\frac{1}{45}x\left(430\,x^2 + \left(-15\sqrt{6} + 600\sqrt{6}\,h_t\right)\,x + 36 + 1\,200h_t^2\right) = 0.$$

The discriminant of the second-order factor is

$$\left(-15\sqrt{6} + 600\sqrt{6}\,h_t\right)^2 - 4\cdot 430\left(36 + 1\,200\,h_t^2\right) = -60\,570 - 108\,000\,h_t + 96\,000\,h_t^2,$$

which is strictly negative for $0 \leq h_t \leq 1$. Thus, the system (3.5.13) has the unique solution $x = y = z = 0$ for $h_t \geq h_*$. $\square$

The proof of Theorem 3.1.2 now follows.

Proof of Theorem 3.1.2. Fix a radius $R \geq 1$ and let h_* be given by Lemma 3.5.5. From Lemma 3.5.1, we can find $\tau_1 = \tau_1(R)$ such that when $t \geq \tau_1$, the inequality $h_t \geq h_*$ holds for $r \in (1, R)$. Let τ_2 be such that

$$\frac{t}{8} \geq \frac{43}{8}\lambda(t) \tag{3.5.16}$$

for $t \geq \tau_2$ (such a τ_2 exists because $\lambda(t) \leq C\sqrt{t}$ for $t \gg 1$). Choose $\alpha = 2/5$, $\beta = 1$ and let $t^* = t^*(2/5, 1)$ be given by Proposition 3.5.4. Finally, set

$$\tau = \tau(R) := \max\{\tau_1(R), \tau_2, t^*\}.$$

We fix $t \geq \tau$, an admissible map $\mathbf{Q} \in W^{1,2}(\Omega, \mathbf{S}_0)$ and we write $\mathbf{Q} = \mathbf{H}_t + \mathbf{V}$. From Equation (3.4.2), we deduce that

$$F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) = \frac{1}{2}\delta^2 F_t(\mathbf{H}_t)\cdot\mathbf{V} + \int_\Omega \left\{ -\frac{\sqrt{6}\lambda(t)}{2}\operatorname{tr}\mathbf{V}^3 + \frac{t+3\lambda(t)}{8}\left(4(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 + \left|\mathbf{V}\right|^4\right)\right\}.$$

Using Proposition 3.5.4 with $\alpha = 2/5$ and $\beta = 1$, we obtain

$$\begin{aligned} F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq \int_\Omega \Bigg\{ & \frac{2\lambda(t)}{5}v_0^2 + \lambda(t)\left(v_3^2 + v_4^2\right) - \frac{\sqrt{6}\lambda(t)}{2}\operatorname{tr}\mathbf{V}^3 \\ & + \frac{3\lambda(t)}{2}(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 + \frac{3\lambda(t)}{8}\left|\mathbf{V}\right|^4 + \frac{t}{8}\left(2(\mathbf{H}_t\cdot\mathbf{V}) + \left|\mathbf{V}\right|^2\right)^2\Bigg\}. \end{aligned} \tag{3.5.17}$$

Clearly, it holds that

$$-\frac{3\lambda(t)}{2}(\mathbf{H}_t\cdot\mathbf{V})\left|\mathbf{V}\right|^2 \geq -\frac{3\lambda(t)}{8}\left(2(\mathbf{H}_t\cdot\mathbf{V}) + \left|\mathbf{V}\right|^2\right)^2. \tag{3.5.18}$$

Combining (3.5.17), (3.5.18) and (3.5.16), we deduce that

$$F_t(\mathbf{Q}) - F_t(\mathbf{H}_t) \geq \lambda(t)\int_\Omega \varphi(\mathbf{V}),$$

where φ is the function defined in Lemma 3.5.5. Since $\varphi \geq 0$ and $\varphi(\mathbf{V}) = 0$ if and only if $\mathbf{V} = 0$, the theorem follows. ☐

3.6 Conclusions

This chapter focuses on the radial-hedgehog solution on a 3D spherical shell, with Dirichlet radial conditions on both spherical concentric boundaries. We define the radial-hedgehog solution by analogy with the definition on a 3D spherical droplet, as used in [71, 51]. We work in the low-temperature regime, with temperatures below the critical nematic supercooling temperature, defined by $t \geq 0$. In Proposition 3.3.1, we construct an explicit sub-solution for the scalar order parameter of the radial-hedgehog solution, h_t, in terms of the shell width $R-1$, independent of t. This sub-solution yields positive lower bounds for h_t, which is sufficient to prove the local stability of the radial-hedgehog solution for sufficiently small $R-1$, in the Landau-de Gennes theoretical framework. In Section 3.4, we prove the global minimality of the radial-hedgehog solution for sufficiently small $R-1$ and for all $t \geq 0$. In Theorem 3.1.1, we provide quantitative information about the required smallness of $R-1$. The main challenge in Theorem 3.1.1 is a quantitative control on the non-quadratic terms in the Landau-de Gennes energy density, which in turn relies on the control over h_t. In particular, we prove that the sum of the non-quadratic terms is non-negative for $R-1$ sufficiently small, so that positivity of the second variation of the Landau-de

Gennes energy (under the hypotheses of Theorem 3.1.1) is equivalent to the global minimality of the radial-hedgehog solution. In Section 3.5, we study the local and global stability of the radial-hedgehog solution for large t. The key point is that $h_t \to 1$ uniformly as $t \to \infty$ for all values of $R-1$. We adapt the arguments in [73] along with the t-control on h_t to derive an improved lower bound for the second variation of the Landau-de Gennes energy. In contrast to Section 3.4, the sum of the non-quadratic terms in the Landau-de Gennes energy density need not be non-negative in the $t \to \infty$ limit. However, their negative contribution can be absorbed by the second variation and this is enough to prove the global minimality of the radial-hedgehog solution in Theorem 3.1.2, in the $t \to \infty$ limit, for all choices of $R-1$.

There has been substantial previous work on the radial-hedgehog solution on a 3D spherical droplet, both analytical and numerical. However, previous analytical work focuses on the second variation of the Landau-de Gennes energy about the radial-hedgehog solution or equivalently, the quadratic contributions to the energy difference, $F_t(\mathbf{Q}) - F_t(\mathbf{H}_t)$, in Equation (3.3.1). We perform a quantitative analysis of the full energy expansion in (3.3.1), for a 3D spherical shell with radial boundary conditions, which allows to prove global minimality results for certain model situations. As stated in the introduction, we believe that our methods give new insight into how the quadratic, cubic and quartic components of the Landau-de Gennes energy density interact with each other.

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La formule de l'indice de Morse pour de champs de vecteurs VMO sur des variétés compactes à bord

Dans ce travail, nous nous intéressons aux champs de vecteurs VMO définis sur des variétés compactes à bord. Inspirés par des travaux de Brezis et Nirenberg [25, 26], nous construisons un invariant topologique — l'indice — pour de tels champs, et nous montrons que cet invariant satisfait une identité, qui dans le cadre continu est connue sous le nom de formule de Morse. Grâce à ces outils, nous pouvons caractériser l'ensemble des données au bord prolongeables à des champs de vecteurs unitaires VMO. Enfin, nous donnons une application de ces notions aux champs de lignes (non orientées) de régularité VMO. Ce dernier résultat possède une interprétation physique naturelle, qui fait intervenir un film mince de nématiques étalés sur une surface.

Ce preprint a été écrit en collaboration avec Antonio Segatti et Marco Veneroni.

Chapter 4

Morse's index formula in VMO for compact manifolds with boundary

Joint work with Antonio Segatti[1] *and Marco Veneroni*[1].

[1] Dipartimento di Matematica "F. Casorati", Università di Pavia, 27100 — Pavia, Italy

Abstract

We study Vanishing Mean Oscillation vector fields on a compact manifold with boundary. Inspired by the work of Brezis and Nirenberg, we construct a topological invariant — the index — for such fields, and establish the analogue of Morse's formula. As a consequence, we characterize the set of boundary data which can be extended to nowhere vanishing VMO vector fields. Finally, we show briefly how these ideas can be applied to (unoriented) line fields with VMO regularity, thus providing a reasonable framework for modeling a surface coated with a thin film of nematic liquid crystals.

Contents

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4.1 Introduction

The starting point of the investigations developed in this chapter is the analysis of a variational model for nematic shells. Nematic shells are the datum of a two-dimensional surface (for simplicity, at a first step, without boundary) $N \subseteq \mathbb{R}^3$ coated with a thin film of nematic liquid crystal ([80, 91, 109, 110, 111, 129, 130, 135]). This line of research has attracted a lot of attention from the physics community due to its vast technological applications (see [111]). From the mathematical point of view, nematic shells offer an interesting and nontrivial interplay between calculus of variations, partial differential equations, geometry and topology. The basic mathematical description of nematic shells consists in an energy defined on tangent vector fields with unit length, named directors. This energy, in the simplest situation, takes the form

$$E(\mathbf{n}) := \frac{1}{2}\int_N |\nabla \mathbf{n}|^2 \mathrm{d}S, \tag{4.1.1}$$

where ∇ stands for the covariant derivative of the surface N. If one is interested in the minimization of this energy, the first step is to understand whether there are competitors for the minimization process. For this type of energy, the natural functional space where to look for minimizers is the space of tangent vector fields with H^1 regularity. This means, recalling that we are looking for vector fields with unit norm, the space defined in this way

$$H^1_{\tan}(N, \mathbb{S}^2) := \left\{\mathbf{n} \in H^1(N, \mathbb{R}^3) : \mathbf{n}(x) \in T_x N \text{ and } |\mathbf{n}| = 1 \text{ a.e.}\right\}. \tag{4.1.2}$$

Now, the problem turns into the understanding of the topological conditions on N, if any, that make $H^1_{\tan}(N, \mathbb{S}^2)$ empty or not. Note that this problem, in the case $N = \mathbb{S}^2$, is indeed a Sobolev version of the celebrated hairy ball problem concerning the existence of a tangent vector field with unit norm on the two-dimensional sphere. The answer, when dealing with continuous fields, is negative. This is a consequence of a more general result, the Poincaré-Hopf Theorem, that relates the existence of a smooth tangent vector field with unit norm to the topology of N. More precisely, a smooth vector field with unit norm exists if and only if $\chi(N) = 0$, where χ is the Euler characteristic of N. In case N is a compact surface in $\mathbb{R}^3$, the Euler characteristic can be written as a function of the topological genus k:

$$\chi(N) = 2(1-k).$$

In [129] it has been proved, using calculus of variations tools, that the very same result holds for vector fields with H^1 regularity. Therefore, up to diffeomorphisms, the only compact surface in $\mathbb{R}^3$ which admits a unit norm vector field in H^1 is the torus, corresponding to $k = 1$. On the other hand, it is easy to comb the sphere with a field $\mathbf{v} \in W^{1,p}_{\tan}(\mathbb{S}^2, \mathbb{S}^2)$ for all $1 \le p < 2$. It is interesting to note that this result could be seen as a "non flat" version of a well know result of Bethuel that gives conditions for the non emptiness of the space

$$H^1_{\mathbf{g}}(\Omega, \mathbb{S}^1) := \left\{\mathbf{v} \in H^1(\Omega, \mathbb{R}^2) \colon |\mathbf{v}(x)| = 1 \text{ a.e. in } \Omega \text{ and } \mathbf{v} = \mathbf{g} \text{ on } \partial\Omega\right\},$$

where Ω is a simply connected bounded domain in $\mathbb{R}^2$ and $\mathbf{g}$ is a prescribed smooth boundary datum with $|\mathbf{g}| = 1$. The non-emptiness of $H^1_{\mathbf{g}}(\Omega, \mathbb{S}^1)$ is related to a topological condition on the Dirichlet datum $\mathbf{g}$ (see [12] and [14]) while in the result in [129] the topological constraint is on the genus of the surface.

Instead of using the standard Sobolev theory, we reformulate this problem in the space of Vanishing Mean Oscillation (VMO) functions, introduced by Sarason in [124], which constitute a special subclass of Bounded Mean Oscillations functions, defined by John and Nirenberg in [77]. We recall the definitions and some properties of these objects in Section 4.2, but we immediately note that VMO contains the critical spaces with respect to Sobolev embeddings, that is,

$$W^{s,p}(\mathbb{R}^n) \subseteq \mathrm{VMO}(\mathbb{R}^n) \qquad \text{when } sp = n,\ 1 < s < n. \tag{4.1.3}$$

In a sense, VMO functions are a good surrogate for the continuous functions, because some classical topological constructions can be extended, in a natural way, to the VMO setting. In particular, we recall here the VMO degree theory, which has been developed after Brezis and Nirenberg's seminal papers [25] and [26].

Besides relaxing the regularity on the vector field, we will consider n-dimensional compact and connected submanifolds of $\mathbb{R}^{n+1}$ and, instead of fixing the length of the vector field to be 1, we will look for vector fields which are bounded and uniformly positive.

Thus, the problem of combing a two-dimensional surface with H^1 vector fields can be generalized in the following way.

Question 1. *Let N be a compact, connected submanifold of $\mathbb{R}^{n+1}$, without boundary, of dimension n. Does a vector field $\mathbf{v} \in \mathrm{VMO}(N, \mathbb{R}^{n+1})$, satisfying*

$$\mathbf{v}(x) \in T_x N \quad \textit{and} \quad c_1 \leq |\mathbf{v}(x)| \leq c_2 \tag{4.1.4}$$

for a.e. $x \in N$ and some constants $c_1, c_2 > 0$, exists?

The first outcome of this work is to provide a complete answer to Question 1. By means of the Brezis and Nirenberg's degree theory, we can show that the existence of nonvanishing vector fields in VMO is subject to the same topological obstruction as in the continuous case, that is, we prove the following

Proposition 4.1.1. *Let N be a compact, connected n-submanifold of $\mathbb{R}^{n+1}$, without boundary. There exists a function $\mathbf{v} \in \mathrm{VMO}(N, \mathbb{R}^{n+1})$ satisfying (4.1.4) if and only if $\chi(N) = 0$.*

After addressing manifolds without boundary, we consider the case where N is a manifold with boundary, and we prescribe Dirichlet boundary conditions to the vector field $\mathbf{v}$ on N. The main issue of this chapter is to understand which are the topological conditions on the manifold N and on the Dirichlet boundary datum that guarantee the existence of a nonvanishing and bounded tangent vector field on N extending the boundary condition. Applications of these results can be found in variational problems for vector fields that satisfy a prescribed boundary condition of Dirichlet type, e.g., in the framework of liquid crystal shells.

More precisely, we address the following problem:

Question 2. *Let $N \subseteq \mathbb{R}^d$ be a compact, connected and orientable n-submanifold with boundary. Let $\mathbf{g}\colon \partial N \to \mathbb{R}^d$ be a boundary datum in* VMO*, satisfying*

$$\mathbf{g}(x) \in T_x N \quad \textit{and} \quad c_1 \leq |\mathbf{g}(x)| \leq c_2 \tag{4.1.5}$$

for $\mathscr{H}^{n-1}$-a.e. $x \in \partial N$ and some constants $c_1, c_2 > 0$. Does a field $\mathbf{v} \in \mathrm{VMO}(N, \mathbb{R}^d)$, which fulfills (4.1.4) *and has trace $\mathbf{g}$ (in some sense, to be specified), exist?*

When working in the continuous setting, a similar issue can be investigated with the help of a topological tool: the index of a vector field. In particular, even in this weak framework, we expect conditions that relate the index of the boundary conditions with the index of the tangent vector field and the Euler characteristic of N. In order to understand the difficulties and to ease the presentation, we recall here some definitions related to the degree theory and an important property.

First, we recall Brouwer's definition of degree. Let N be as in Question 2 and let M be a connected, orientable manifold without boundary, of the same dimension as N. Let $\varphi\colon N \to M$ be a smooth map, and let $p \in M \setminus \varphi(\partial N)$ be a regular value for φ (that is, the Jacobian matrix $D\varphi(x)$ is non-singular for all $x \in \varphi^{-1}(p)$). We define the degree of φ with respect to p as

$$\deg(\varphi, N, p) := \sum_{x \in \varphi^{-1}(p)} \mathrm{sign}(\det D\varphi(x)).$$

This sum is finite, because $\varphi^{-1}(p)$ is a discrete set (as φ is locally invertible around each point of $\varphi^{-1}(p)$) and N is compact.

It can be proved that, if p_1 and p_2 are two regular values in the same component of $M \setminus \varphi(\partial N)$, then $\deg(\varphi, N, p_1) = \deg(\varphi, N, p_2)$. Since the regular values of φ are dense in M (by Sard lemma), the definition of $\deg(\varphi, N, p)$ can be extended to every $p \in M \setminus \varphi(\partial N)$. Moreover, by approximation it is possible to the define the degree when φ is just continuous. In case N is a manifold without boundary,

$\deg(\varphi, N, p)$ does not depend on the choice of $p \in M$, so we will denote it by $\deg(\varphi, N, M)$. Let us mention also that, if N and M are compact and without boundary, the following formula holds:

$$\deg(\varphi, N, M) = \frac{1}{\tau(M)} \int_N \varphi^*(\mathrm{d}\tau) = \frac{1}{\tau(M)} \int_N \det D\varphi(x)\,\mathrm{d}\sigma(x), \tag{4.1.6}$$

where σ, τ are the Riemannian metrics on N and M, respectively.

Ideally, given a continuous vector field $\mathbf{v}$, one would like to define its index by

$$\operatorname{ind}(\mathbf{v}, N) = \deg(\mathbf{v}, N, 0).$$

However, this is not possible, because in order to define the degree it is essential that the domain and the target manifold have the same dimension. This is not the case here, since the domain manifold $N \subseteq \mathbb{R}^d$ has dimension strictly less that the target manifold $\mathbb{R}^d$. To overcome this issue, there are at least two different strategies. The one we consider in this chapter, which is also the most widely studied in the literature (see, e.g., [59, 90, 101, 106, 134]), is to use coordinate charts to represent $\mathbf{v}$, locally around its zeros, as a map $\mathbb{R}^n \to \mathbb{R}^n$. This requires an additional assumption, namely that the zero set of $\mathbf{v}$ is discrete. Thus, within this approach, an approximation technique is needed in order to extend the definition of index to any continuous field. This construction, based on the Transversality Theorem, is explained in detail in Section 4.3. Another possibility is to consider an open neighborhood $U \subseteq \mathbb{R}^d$ of N, and extend $\mathbf{v}$ to a map $\mathbf{w}\colon U \to \mathbb{R}^d$, in a suitable way. Then, it would make sense to write

$$\operatorname{ind}(\mathbf{v}, N) := \deg(\mathbf{w}, U, 0),$$

and this would give an equivalent definition of the index. This approach is inspired by a classical proof of the Poincaré-Hopf theorem, which can be found in [101, Theorem 1, p. 38]). Some details of this construction are given in Remark 4.3.1.

Once the index has been properly defined, it can been used to establish a precise relation between the behaviour of a vector field $\mathbf{v}$ and the topological properties of N. Denote by $\partial_- N$ the subset of the boundary where $\mathbf{v}$ points inward (that is, letting $\nu(x)$ be the outward unit normal to ∂N in $T_x N$, we have $x \in \partial_- N$ if and only if $\mathbf{v}(x) \cdot \nu(x) < 0$). Call $P_{\partial N}\mathbf{v}$ the vector field on ∂N defined by

$$P_{\partial N}\mathbf{v}(x) := \operatorname{proj}_{T_x \partial N} \mathbf{v}(x) \qquad \text{for all } x \in \partial N.$$

Morse proved the following equality (see [106]), which was later rediscovered and generalized by Pugh (see [116]) and Gottlieb (see [56, 57]).

Proposition 4.1.2 (Morse's index formula)**.** *If $\mathbf{v}$ is a* continuous *vector field over N satisfying $0 \notin \mathbf{v}(\partial N)$, with finitely many zeros, and if $P_{\partial N}\mathbf{v}$ has finitely many zeros, then*

$$\operatorname{ind}(\mathbf{v}, N) + \operatorname{ind}(P_{\partial N}\mathbf{v}, \partial_- N) = \chi(N), \tag{4.1.7}$$

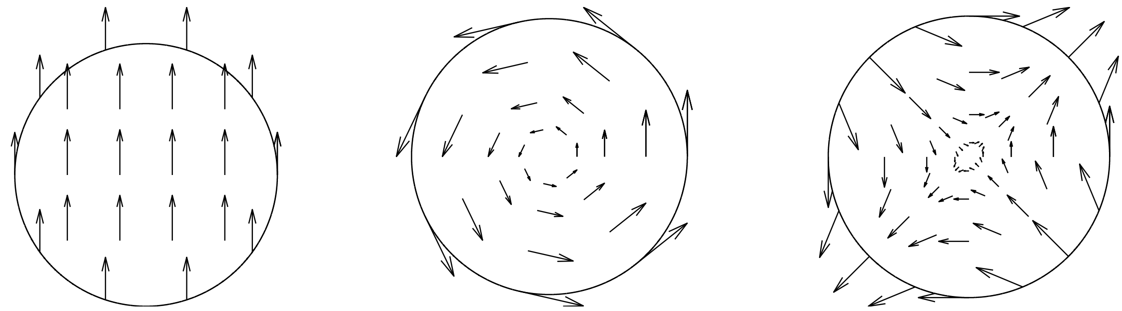
where $\chi(N)$ is the Euler characteristic of N.

In figure 4.1 we plot some examples on $N = \overline{B_r(0)}$. In this case $\chi(N) = 1$.

Identity (4.1.7) can be seen as a generalization of the Poincaré-Hopf index formula. As an immediate corollary, we obtain a necessary condition for the existence of nowhere vanishing vector fields which extends in N a given a boundary datum.

Corollary 4.1.3. *Let $\mathbf{g}\colon \partial N \to \mathbb{R}^d$ be a* continuous *function, satisfying* (4.1.5)*, and assume that $P_{\partial N}\mathbf{g}$ has finitely many zeros. If there exists a* continuous *vector field $\mathbf{v}$, satisfying* (4.1.4)*, such that $\mathbf{v}_{|\partial N} = \mathbf{g}$ then*

$$\operatorname{ind}(P_{\partial N}\mathbf{g}, \partial_- N) = \chi(N).$$



a) $\mathbf{v}_1(x, y) = (0, 1)$ b) $\mathbf{v}_2(x, y) = (-y, x)$ c) $\mathbf{v}_3(x, y) = (y, x)$

Figure 4.1: a) $\mathrm{ind}(\mathbf{v}_1, N) = 0$, $\mathrm{ind}(P_{\partial N}\mathbf{v}_1, \partial_- N) = 1$; b) $\mathrm{ind}(\mathbf{v}_2, N) = 1$, $\mathrm{ind}(P_{\partial N}\mathbf{v}_2, \partial_- N) = 0$; c) $\mathrm{ind}(\mathbf{v}_3, N) = -1$, $\mathrm{ind}(P_{\partial N}\mathbf{v}_3, \partial_- N) = 2$.

This Corollary gives an answer to Question 2 in case we consider smooth vector fields.

Our aim is to extend Proposition 4.1.2 to the VMO setting. For this purpose, we extend the definition of index to arbitrary VMO fields, with a trace at the boundary. We introduce another quantity, which we call "inward boundary index" and denote by $\mathrm{ind}_-(\mathbf{v}, \partial N)$, playing the role of $\mathrm{ind}(P_{\partial N}\mathbf{v}, \partial_- N)$. (The reader is referred to Section 4.4 for the definitions).

Then, our main result is

Theorem 4.1.4. *Let N be a compact, connected and orientable submanifold of $\mathbb{R}^d$, with boundary. Let $\mathbf{g} \in \mathrm{VMO}(\partial N, \mathbb{R}^d)$ be a boundary datum which fulfills*

$$\mathbf{g}(x) \in T_x N \qquad \text{and} \qquad c_1 \leq |\mathbf{g}(x)| \leq c_2$$

for some constants c_1, $c_2 > 0$ and $\mathscr{H}^{n-1}$-a.e. $x \in \partial N$. If $\mathbf{v} \in \mathrm{VMO}(N, \mathbb{R}^d)$ is a map with trace $\mathbf{g}$ at the boundary, satisfying

$$\mathbf{v}(x) \in T_x N$$

for a.e. $x \in N$, then

$$\mathrm{ind}(\mathbf{v}, N) + \mathrm{ind}_-(\mathbf{v}, \partial N) = \chi(N).$$

Note that this Theorem is the analogous of Proposition 4.1.2 for VMO vector fields. Finally, regarding Question 2, we have the following answer.

Proposition 4.1.5. *Let $\mathbf{g} \in \mathrm{VMO}(\partial N, \mathbb{R}^d)$ satisfy* (4.1.5)*. A field $\mathbf{v} \in \mathrm{VMO}(N, \mathbb{R}^d)$ that satisfies the condition* (4.1.4) *and has trace $\mathbf{g}$ exists if and only if*

$$\mathrm{ind}_-(\mathbf{g}, \partial N) = \chi(N). \tag{4.1.8}$$

In case the boundary datum satisfies (4.1.5), (4.1.8) and $\mathbf{g} \in W^{1-1/p,p}(\partial N, \mathbb{R}^d)$ for some $1 < p < +\infty$, one can choose an extension $\mathbf{v}$ which, in addition to (4.1.4), satisfies $\mathbf{v} \in W^{1,p}(N, \mathbb{R}^d)$ (see Corollary 4.4.6). Therefore, the results we discuss in this chapter are indeed relevant to the analysis of variational models for nematic shells.

We conclude this introduction with an outline of the chapter. In Section 4.2 we provide some preliminary material on the VMO space. Then, in Section 4.3 we introduce the notion of index for a continuous vector field, starting with the basic case of a field with a finite number of zeros and then moving to an arbitrary number of zeros by Thom's Transversality Theorem. In Section 4.4, by means of an approximation argument, this extension allows us to give a notion of index for a VMO vector field and to prove Theorem 4.1.4. Finally, in Section 4.5, we apply these results to the existence of line fields with VMO regularity. Interestingly, such an existence result shares the same topological obstruction as the existence result for vector fields. As a side result of the existence of VMO Q-tensor fields, we obtain topological conditions for the existence of line fields with VMO regularity, thus extending to this weaker setting a classical result due to Poincaré and Kneser.

Notation. In the following sections either $N = \mathbb{R}^n$, or N is a compact, connected and oriented manifold with boundary, of dimension n, embedded as a submanifold of $\mathbb{R}^d$ for some $d \in \mathbb{N}$.

- The injectivity radius of N (see, e.g., do Carmo [43]) is called r_0.
- We denote geodesic balls in N by $B_r^N(x)$ or simply $B_r(x)$, when it is clear from the context that we work in N. In case $N = \mathbb{R}^n$, we write $B_r^n(x)$ or $B^n(x, r)$.
- For $\varepsilon > 0$, we set
$$N_\varepsilon := \{x \in N \colon \operatorname{dist}(x, \partial N) \geq \varepsilon\}.$$
- For each $x \in \partial N$, we denote by $\nu(x)$ the outward unit normal to ∂N in $T_x N$.
- Given a non-empty, convex and closed set $K \subseteq \mathbb{R}^d$, we denote the nearest-point projection on K by proj_K.
- Given a manifold $X \subseteq \mathbb{R}^d$ and a continuous map $\mathbf{v} \colon X \to \mathbb{R}^d$, we denote the tangential component of $\mathbf{v}$ by
$$P_X \mathbf{v}(x) := \operatorname{proj}_{T_x X} \mathbf{v}(x) \qquad \text{for } x \in X.$$

4.2 Preliminary material: VMO functions

For the reader's convenience, we recall here the basic definitions about VMO functions, following the presentation of [26] (to which the reader is referred, for more details). All the functions we consider here take values in $\mathbb{R}^d$, so functional spaces such as, e.g., $L^1(N, \mathbb{R}^d)$ or $\mathrm{VMO}(N, \mathbb{R}^d)$ will be simply written as $L^1(N)$ or $\mathrm{VMO}(N)$.

Recall that N is endowed with a Riemannian measure σ. For $\mathbf{u} \in L^1(N)$ (with respect to σ), define

$$\|u\|_{\mathrm{BMO}} := \sup_{\varepsilon \leq r_0,\, x \in N_{2\varepsilon}} \fint_{B_\varepsilon(x)} |\mathbf{u}(y) - \bar{\mathbf{u}}_\varepsilon(x)| \, \mathrm{d}\sigma(y), \tag{4.2.1}$$

where

$$\bar{\mathbf{u}}_\varepsilon(x) := \fint_{B_\varepsilon(x)} \mathbf{u}(y) \, \mathrm{d}\sigma(y), \qquad \text{for } x \in N_{2\varepsilon}. \tag{4.2.2}$$

The set of functions with $\|\mathbf{u}\|_{\mathrm{BMO}} < +\infty$ will be denoted $\mathrm{BMO}(N)$, and (4.2.1) defines a norm on $\mathrm{BMO}(N)$ modulo constants. Using cubes instead of balls leads to an equivalent norm. Moreover, if $\varphi \colon X_1 \to X_2$ is a C^1 diffeomorphism between two unbounded manifolds, then $\mathbf{u} \in \mathrm{BMO}(X_2)$ implies $\mathbf{u} \circ \varphi \in \mathrm{BMO}(X_1)$ and
$$\|\mathbf{u} \circ \varphi\|_{\mathrm{BMO}(X_1)} \leq C \, \|\mathbf{u}\|_{\mathrm{BMO}(X_2)}.$$
Bounded functions (in particular, continuous functions) belong to BMO. Following Sarason, we define $\mathrm{VMO}(N)$ as the closure of $C^0(N)$ with respect to the BMO norm. Functions in $\mathrm{VMO}(N)$ can be characterized by means of this lemma (see [25, Lemma 3]):

Lemma 4.2.1. *A function* $\mathbf{u} \in \mathrm{BMO}(N)$ *is in* $\mathrm{VMO}(N)$ *if and only if*

$$\lim_{\varepsilon \to 0} \sup_{x \in N_{2\varepsilon}} \fint_{B_\varepsilon(x)} |\mathbf{u}(y) - \bar{\mathbf{u}}_\varepsilon(x)| \, \mathrm{d}\sigma(y) \to 0.$$

Sobolev spaces provide an interesting class of functions in VMO, since, for critical exponents, the embeddings which fail to be in L^∞ hold true in VMO:

$$W^{s,p}(N) \subseteq \mathrm{VMO}(N) \qquad \text{whenever } 0 < s < n,\ sp = n.$$

In general, VMO functions do not have a trace on the boundary. However, it is possible to introduce a subclass of VMO for which traces are well defined. We sketch here the construction.

First, we need to embed N as a domain of a bigger manifold X, smooth and without boundary. Here, we take X as the double of N, that is, the manifold we obtain by gluing two copies of N along their boundaries. Modifying, if necessary, the value of d we can assume that $X \subseteq \mathbb{R}^d$. Also, let U be a tubular neighborhood of ∂N in X, and assume that the nearest-point projection $\pi\colon U \to \partial N$ is well defined. Now, we fix $\mathbf{g} \in \mathrm{VMO}(\partial N)$ and we extend it to a function $\mathbf{G}$, by the formula

$$\mathbf{G}(x) := \begin{cases} \mathbf{g}(\pi(x))\chi(x) & \text{if } x \in X \cap U \\ 0 & \text{if } x \in X \setminus U \end{cases} \tag{4.2.3}$$

where χ is a cut-off function, which is equal to 1 near ∂N and vanishes outside U. It can be checked that $\mathbf{G} \in \mathrm{VMO}(X)$.

We say that a function $\mathbf{u} \in \mathrm{VMO}(N)$ has trace $\mathbf{g}$ on ∂N, and we write $\mathbf{u} \in \mathrm{VMO}_{\mathbf{g}}(N)$, if and only if the function defined by

$$\begin{cases} \mathbf{u} & \text{in } N \\ \mathbf{G} & \text{in } X \setminus N \end{cases}$$

is in $\mathrm{VMO}(X)$. This definition is independent on the choice of χ and of X (see [26, Property 6]). The notion of $\mathrm{VMO}_{\mathbf{g}}$ is stable under diffeomorphism: suppose $\varphi\colon X_1 \to X_2$ is a C^1 diffeomorphism between bounded manifolds, mapping diffeomorphically ∂X_1 onto ∂X_2 . If $\mathbf{g} \in \mathrm{VMO}(\partial X_2)$ and $\mathbf{u} \in \mathrm{VMO}_{\mathbf{g}}(X_2)$, then

$$\mathbf{u} \circ \varphi \in \mathrm{VMO}_{\mathbf{g}\circ\varphi}(X_1).$$

As an example of VMO functions with trace, let us mention that every map in $W^{1,n}(X)$ has a trace in the sense of VMO, which coincides with the Sobolev trace.

4.2.1 Combing an unbounded manifold in VMO

In this section, we prove Proposition 4.1.1. Of course, it could be obtained as a corollary of our main result, Theorem 4.1.4. Anyway, it can be proved independently, and we present here an elementary argument inspired by [64, Theorem 2.28]. We assume that N is a compact, connected n-manifold *without boundary*, embedded as an hypersurface of $\mathbb{R}^{n+1}$.

Proof of Proposition 4.1.1. It is well-known that, if $\chi(N) = 0$, then a nowhere vanishing, smooth (hence VMO) vector field on N exists. The idea of the proof is the following: One picks an arbitrary continuous field, approximates it with a field $\mathbf{v}$ having a finite number of zeros, then uses the Poincaré-Hopf formula and the hypothesis $\chi(N) = 0$ to show that $\mathrm{ind}(\mathbf{v},\, N) = 0$, so $\mathbf{v}$ can be modified into a nowhere vanishing field. This argument is given in detail in the proof of Proposition 4.1.5, in case N is a manifold with boundary, and it is even simpler when $\partial N = \emptyset$.

Let us prove the other side of the proposition: we suppose that a tangent vector field $\mathbf{v} \in \mathrm{VMO}(N)$ such that $\operatorname{ess\,inf}_N |\mathbf{v}| > 0$ exists, and we claim that $\chi(N) = 0$. Every compact hypersurface of $\mathbb{R}^{n+1}$ is orientable, so there is a smooth unit vector field $\gamma\colon N \to \mathbb{R}^{n+1}$ such that $\gamma(x) \perp T_x N$ for all $x \in N$. The choice of such a map induces an orientation on N, and γ is called the Gauss map of the oriented manifold N. We can also assume that n is even, since $\chi(N) = 0$ whenever N is a compact, unbounded manifold of odd dimension (see, e.g., [64, Corollary 3.37]).

Consider the function $H\colon N \times [0,\, \pi] \to \mathbb{R}^{n+1}$ given by

$$H(x,\, t) := (\cos t)\gamma(x) + (\sin t)\frac{\mathbf{v}(x)}{|\mathbf{v}(x)|}.$$

It is readily checked that $|H(x,t)|^2 = 1$ for all $(x,t) \in N \times [0,\, \pi]$. We claim that

$$H \in C^0\left([0,\, \pi],\, \mathrm{VMO}(N,\, \mathbb{S}^n)\right). \tag{4.2.4}$$

Indeed, $H(\cdot, t)$ is the linear combination of functions in $\mathrm{VMO}(N)$ and hence belongs to $\mathrm{VMO}(N)$, for all t. On the other hand, for all $t_1,\, t_2 \in [0, \pi]$

$$\|H(\cdot,\, t_1) - H(\cdot,\, t_2)\|_{\mathrm{BMO}} \le |\cos t_1 - \cos t_2|\, \|\gamma\|_{\mathrm{BMO}} + |\sin t_1 - \sin t_2|\, \|\mathbf{v}\|_{\mathrm{BMO}}\,,$$

whence the claimed continuity (4.2.4) follows.

Since the degree is a continuous function $\mathrm{VMO}(N,\, \mathbb{S}^n) \to \mathbb{Z}$ (see [25, Theorem 1]), we infer that

$$\deg(H(\cdot,\, 0),\, N,\, \mathbb{S}^n) = \deg(H(\cdot,\, \pi),\, N,\, \mathbb{S}^n).$$

On the other hand, $H(\cdot,\, 0) = \gamma$ and $H(\cdot,\, \pi) = -\gamma$. By standard properties of the degree (in particular, [64, Properties (d, f) p. 134]), and since we have assumed that n is even, we have

$$\deg(-\gamma,\, N,\, \mathbb{S}^n) = (-1)^{n+1} \deg(\gamma,\, N,\, \mathbb{S}^n) = -\deg(\gamma,\, N,\, \mathbb{S}^n),$$

hence

$$\deg(\gamma,\, N,\, \mathbb{S}^n) = -\deg(\gamma,\, N,\, \mathbb{S}^n).$$

By the degree formula (4.1.6) and Gauss-Bonnet Theorem (see, e.g., [59, page 196]), for an even-dimensional hypersurface N there holds

$$\deg(\gamma,\, N,\, \mathbb{S}^n) = \deg(\gamma,\, N,\, \mathbb{S}^n) \fint_{\mathbb{S}^n} \mathrm{d}\sigma_n = \frac{1}{\omega_n}\int_N \gamma^*(\mathrm{d}\sigma_n) = \frac{1}{\omega_n}\int_N \kappa \,\mathrm{d}\sigma = \frac{1}{2}\chi(N),$$

where $\mathrm{d}\sigma_n$ is the volume form of $\mathbb{S}^n$, $\omega_n := \int_{\mathbb{S}^n} \mathrm{d}\sigma_n$ is the volume of $\mathbb{S}^n$, and κ is the Gaussian curvature of N. Since $\deg(\gamma,\, N,\, \mathbb{S}^n) = 0$ by the above construction, this shows that $\chi(N) = 0$ and thus completes the proof. $\square$

Remark 4.2.1. When $\chi(N) \neq 0$, Proposition 4.1.1 shows that there is no unit vector field in the critical Sobolev space $W^{s,p}(N)$, for $0 < s < n$ and $sp = n$. In contrast, when $sp < n$ it is not difficult to construct unit vector fields in $W^{s,p}(N)$. For instance, on $N = \mathbb{S}^{2k}$ one may consider a field with two "hedgehog" singularities, of the form $x \mapsto x/\,|x|$, located at the opposite poles of the sphere.

4.3 The index of a continuous field

We aim to extend Morse formula to the VMO setting. As a preliminary step, we need to define the index for any continuous vector field, dropping out the assumption of finitely many zeros. This goal can be achieved quite straightforwardly, by applying a fundamental tool of differential geometry: the transversality theorem. Such a construction is usually given for granted but, for the reader's convenience, in this section we present it in detail. As a consequence of the transversality theorem, we are able to extend some properties of the classical index of a vector field, namely excision, invariance under homotopy, and stability, to continuous vector fields with any number of zeros. In Propositions 4.3.4 and 4.3.5 and in Corollary 4.3.6 we give the corresponding statements.

Let us start by recalling the definition of transversality. Throughout this section, we denote by $X \subseteq \mathbb{R}^d$ a compact, connected and oriented manifold without boundary (in what follows we will take as X either the double of N or ∂N). Also, let E be a smooth manifold (without boundary), $\varphi\colon X \to E$ a map of class C^1, and $Y \subseteq E$ a submanifold.

Definition 4.3.1. The map φ is said to be transverse to Y if and only if, for all $x \in \varphi^{-1}(Y)$, we have

$$\mathrm{d}\varphi_x(T_x X) + T_{\varphi(x)}Y = T_{\varphi(x)}E.$$

In other words, we ask the image of φ to "cross transversally" the submanifold Y, at each point of intersection. In our case of interest, $E = TX$ is the tangent bundle of X, equipped with the natural projection $\pi\colon E \to X$ given by $(x, \mathbf{w}) \mapsto x$. We take φ to be a section of π — that is, a map $\varphi\colon X \to E$ such that $\pi \circ \varphi = \mathrm{Id}_X$.

There is a natural bijection between sections of π and vector fields, i.e. maps $\mathbf{v}\colon X \to \mathbb{R}^d$ which satisfy $\mathbf{v}(x) \in T_x N$ for any $x \in X$. For each section φ can be written in the form

$$\varphi(x) = (x, \mathbf{v}(x)) \qquad \text{for all } x \in X$$

for a unique vector field $\mathbf{v}$, which is as regular as φ. Conversely, given $\mathbf{v}$ this formula uniquely defines a section φ of π. Finally, we take Y as the image of the zero section, that is,

$$Y := \{(x, 0)\colon x \in X\} \subset E.$$

Clearly, Y is a submanifold of E, diffeomorphic to X, and $\varphi(x) \in Y$ if and only if $v(x) = 0$.

Fix a point $x \in X$ and consider a chart $f\colon V \to \mathbb{R}^n$ defined in an open neighborhood V of x. The map f naturally induces a chart $F\colon TV \to \mathbb{R}^{2n}$ of TX, by setting $F(y, \mathbf{v}) := (f(y), \mathrm{d}f_y(\mathbf{v}))$ for any $y \in V$ and $\mathbf{v} \in T_y X$. Let $f_*\mathbf{v}\colon f(V) \subset \mathbb{R}^n \to \mathbb{R}^n$ be defined by

$$f_*\mathbf{v}(y) := \mathrm{d}f_{f^{-1}(y)}\left(\mathbf{v} \circ f^{-1}(y)\right) \qquad \text{for } y \in f(V) \subset \mathbb{R}^n.$$

Then, there holds

$$\left(F \circ \varphi \circ f^{-1}\right)(z) = (z, f_*\mathbf{v}(z)) \qquad \text{for } z \in f(V) \subset \mathbb{R}^n$$

and, by interpreting Definition 4.3.1 through the chart F, we deduce the

Proposition 4.3.1. *The map φ is transverse to Y if and only if for all $x \in \mathbf{v}^{-1}(0)$ the differential $\mathrm{d}(f_*\mathbf{v})_{f(x)}$ is invertible.*

If f, g are two local charts around x, then $\mathrm{d}(f_*\mathbf{v})_{f(x)}$ is invertible if and only if $\mathrm{d}(g_*\mathbf{v})_{g(x)}$ is, so this characterization is independent of the choice of the chart. Vector fields in these conditions will simply be called transverse fields. Remark that, for a transverse field $\mathbf{v}$, the set $\mathbf{v}^{-1}(0)$ is discrete (by the local inversion theorem), hence is finite because X is compact. Moreover, given two coordinate charts f and g which agree with the fixed orientation of X, the Jacobians $\det \mathrm{d}(f_*\mathbf{v})_{f(x)}$ and $\det \mathrm{d}(g_*\mathbf{v})_{g(x)}$ have the same sign. Thus, if $U \subseteq X$ is an open set and $\mathbf{v}$ a transverse vector field on X satisfying

$$0 \notin \mathbf{v}(\partial U),$$

the index of $\mathbf{v}$ on U is well-defined by the formula

$$\operatorname{ind}(\mathbf{v}, U) := \sum_{x \in \mathbf{v}^{-1}(0) \cap U} \operatorname{sign} \det \mathrm{d}(f_*\mathbf{v})_{f(x)}. \tag{4.3.1}$$

This formula can be expressed in an equivalent way. Pick a geodesic ball $B_r(x) \subset\subset U$ around each zero x, so small that no other zero is contained in $B_r(x)$. Then, $|f_*\mathbf{v}|^{-1} f_*\mathbf{v}$ is well-defined as a map $\partial B_r(x) \simeq \mathbb{S}^{n-1} \to \mathbb{S}^{n-1}$, and

$$\operatorname{ind}(\mathbf{v}, U) = \sum_{x \in \mathbf{v}^{-1}(0) \cap U} \deg\left(\frac{f_*\mathbf{v}}{|f_*\mathbf{v}|},\, \partial B_r(x),\, \mathbb{S}^{n-1}\right). \tag{4.3.2}$$

The equivalence of (4.3.1) and (4.3.2) follows, e.g., from [26, Equation (4.1), p. 25].

Since we want to extend the definition of index to any continuous field, it is natural to ask whether a continuous field can be approximated by transverse fields. The transversality theorem gives a positive answer. This result, due to Thom (see [137, 138]), states that transverse mappings are a dense subset of continuous mappings. The statement that we present here is [27, Theorem 14.6]. This formulation is convenient for our purposes, because it guarantees that if φ is a section of π, then the approximating transverse maps can be chosen to be sections as well.

Theorem 4.3.2 (Transversality theorem). *Let $\pi\colon E \to X$ be a smooth vector bundle, Y a submanifold of E, and $\varphi\colon X \to E$ a smooth section of π. Then, given any continuous function $\varepsilon\colon X \to (0, +\infty)$, there exists a section ψ of π which is transverse to Y and satisfies*

$$\|\varphi(x) - \psi(x)\|_{T_x E} \leq \varepsilon(x) \qquad \text{for all } x \in X.$$

Moreover, if $A \subseteq X$ is a closed set such that $\varphi_{|A}$ is of class C^1 and transverse to Y, then one can choose ψ so that $\psi_{|A} = \varphi_{|A}$.

The smoothness assumption on φ is not really a restriction, because every continuous section can be approximated with smooth sections (e.g., working in coordinate charts which trivialize π). Hence, from this theorem we immediately obtain the result we need about vector fields.

Corollary 4.3.3. *Let U be an open subset of X, and let $\mathbf{v}$ be a continuous vector field defined on $\overline{U}$. If $\mathbf{v}$ satisfies $0 \notin \mathbf{v}(\partial U)$, then there exists a transverse field $\mathbf{u}$ on $\overline{U}$, such that*

$$\text{(4.3.3)} \qquad \mathbf{u} \text{ has finitely many zeros},$$

$$\text{(4.3.4)} \qquad \sup_{x\in\overline{U}} |\mathbf{v}(x) - \mathbf{u}(x)| < \inf_{x\in\partial U} |\mathbf{v}(x)| .$$

Now we can define the index of an arbitrary field.

Definition 4.3.2. Let $\mathbf{v}$ be a continuous vector field on U, such that $0 \notin \mathbf{v}(\partial U)$. If $\mathbf{v}$ is transverse, we define $\mathrm{ind}(\mathbf{v}, U)$ by formula (4.3.1). Otherwise, we define

$$\mathrm{ind}(\mathbf{v}, U) := \mathrm{ind}(\mathbf{u}, U),$$

where $\mathbf{u}$ is any transverse field satisfying (4.3.4).

The well-posedness of this definition follows directly from the the homotopy invariance of the index for transverse vector fields, and can be proved by arguing exactly as for Corollary 4.3.6.

The definition of index closely resembles Brouwer's construction of the degree. This similarity is not coincidental. Indeed, as we mentioned in the Introduction, an equivalent way of making sense of the index for an arbitrary continuous field is to define it as the degree of an appropriate map.

Remark 4.3.1. More precisely, consider a tubular neighborhood $M \subseteq \mathbb{R}^d$ of the manifold X, i.e., an open neighborhood of X in $\mathbb{R}^d$ such that any point $y \in M$ can be uniquely decomposed as $y = x + \nu$, where $x \in X$ and ν is orthogonal to T_xX. Let $\tau\colon M \to X$ be the map given by $y \mapsto x$, which is smooth if M is small enough. Consider the normal extension of $\mathbf{v}$, that is, the continuous function $\mathbf{w}\colon M \to \mathbb{R}^d$ given by

$$\mathbf{w}(y) := \mathbf{v}(\tau(y)) + y - \tau(y) \qquad \text{for all } y \in M.$$

Then, we can set

$$\text{(4.3.5)} \qquad \mathrm{ind}(\mathbf{v}, U) := \deg(\mathbf{w}, \tau^{-1}(U), 0).$$

It is not hard to see that this quantity coincides with the index in the sense of Definition 4.3.2. Actually, by means of Brezis and Nirenberg degree theory, the right-hand side in this formula makes sense when $\mathbf{v}$ is just VMO (and satisfies a suitable nonvanishing condition near the boundary). Thus, one could consider taking (4.3.5) as a general definition of index. However, for a VMO field $\mathbf{v}$ this approach does not allow to define the quantity $\mathrm{ind}_-(P_{\partial N}\mathbf{v}, \partial_- N[\mathbf{v}])$, which occurs in Morse's formula, because $\partial_- N[\mathbf{v}]$ may not be open. Henceforth, one would still have to consider continuous fields at first, then take care of the VMO case by an approximation procedure.

Due to this strong link between the index and the degree, it is not surprising that some important properties of the degree have a counterpart for the index. The first property we consider here is excision.

Proposition 4.3.4 (Excision)**.** *Let $U_1 \subseteq U$, $U_2 \subseteq U$ be two disjoint open sets in X, and let $\mathbf{v}$ be a continuous vector field on X. If $0 \notin \mathbf{v}(\overline{U} \setminus (U_1 \cup U_2))$, then*

$$\operatorname{ind}(\mathbf{v},\, U) = \operatorname{ind}(\mathbf{v},\, U_1) + \operatorname{ind}(\mathbf{v},\, U_2).$$

Proof. Using Theorem 4.3.2, we construct a transverse field $\mathbf{u}$ which satisfies

$$\sup_{x\in N} |\mathbf{v}(x) - \mathbf{u}(x)| < \inf_{x\in\overline{U}\setminus(U_1\cup U_2)} |\mathbf{v}(x)|\,.$$

In particular, $\mathbf{u}$ vanishes nowhere on $\overline{U} \setminus (U_1 \cup U_2)$. By Formula (4.3.1), which defines the index for a transverse field, we deduce

$$\operatorname{ind}(\mathbf{u},\, U) = \operatorname{ind}(\mathbf{u},\, U_1) + \operatorname{ind}(\mathbf{u},\, U_2),$$

hence the lemma is proved. ☐

The second property is the invariance of the index under a continuous homotopy. We state a first version of this principle, in which we allow both the vector field and the underlying domain to vary continuously.

Proposition 4.3.5 (General homotopy principle)**.** *Let $\{M_t\}_{0\le t\le 1}$ be a family of compact, oriented n-manifolds in $\mathbb{R}^d$, without boundary, such that the set*

$$M := \coprod_{0\le t\le 1} M_t \times \{t\}$$

is a $(n+1)$-submanifold of $\mathbb{R}^d \times [0,\,1]$. Let V be an open, connected subset of M, and set $V_t := V \cap (\mathbb{R}^d \times \{t\})$. Let $\mathbf{v}\colon \overline{V} \to \mathbb{R}^d$ be a continuous map such that, for each $0 \le t \le 1$,

(i) $\mathbf{v}(\cdot,\, t)$ *is a tangent field to M_t, and*

(ii) $0 \notin \mathbf{v}(\partial V_t)$.

Then, for any $0 \le t_1,\, t_2 \le 1$ such that $V_{t_1} \neq \emptyset$, $V_{t_2} \neq \emptyset$, we have

$$\operatorname{ind}(\mathbf{v}(\cdot,\, t_1),\, V_{t_1}) = \operatorname{ind}(\mathbf{v}(\cdot,\, t_2),\, V_{t_2}).$$

Proof. Without loss of generality, we assume $t_1 = 0$, $t_2 = 1$. Then, the assumption $V_0 \neq \emptyset$, $V_1 \neq \emptyset$ and the connectedness of V ensure that $V_t \neq \emptyset$ for all $0 < t < 1$. Using (ii) and the transversality theorem, we can take two smooth, transverse fields $\mathbf{u}_0$, $\mathbf{u}_1$, satisfying

$$\sup_{x\in V_i} |\mathbf{u}_i(x) - \mathbf{v}(x,\, i)| < \inf_{x\in\partial V_i} |\mathbf{v}(x,\, i)|$$

for $i \in \{0,\, 1\}$. Moreover, we introduce the sets

$$E := \coprod_{0\le t\le 1} TM_t \times \{t\},$$

$$Y := \{(x,\, 0,\, t)\colon 0 \le t \le 1,\, x \in M_t\} \subseteq E$$

and the map $\pi\colon E \to M$, by setting

$$\pi(x,\, \mathbf{w},\, t) := (x,\, t) \qquad \text{for all } 0 \le t \le 1,\, x \in M_t,\, \mathbf{w} \in T_xM_t.$$

Then, E is a vector bundle over M, with fiber $\mathbb{R}^n$ (remark: $E \neq TM$!), and Y is a submanifold of E. Moreover, thanks to our assumption (i), the function $\varphi\colon V \to E$ given by

$$\varphi(x,\, t) := (x,\, \mathbf{v}(x,\, t),\, t)$$

is a continuous section of π, and $\varphi(x,\, t) \in Y$ if and only if $\mathbf{v}(x,\, t) = 0$. By smoothing $\mathbf{v}$, then applying the transversality theorem as we did in the proof of Corollary 4.3.3, we approximate $\mathbf{v}$ by a section $\psi\colon V \to E$ which is transverse to Y. Denoting by $\mathbf{u}(\cdot,\, t)$ the vector field on V_t induced by $\psi(\cdot,\, t)$, we can assume that

$$\sup_{x\in\overline{V}_t} |\mathbf{u}(x,\, t) - \mathbf{v}(x,\, t)| < \inf_{x\in\partial V_t} |\mathbf{v}(x,\, t)| \qquad \text{for all } 0 \leq t \leq 1$$

(which is possible, thanks to (ii)) and that $\mathbf{u}(\cdot,\, i) = \mathbf{u}_i$ for $i \in \{0,\, 1\}$ (because $\mathbf{u}_0$, $\mathbf{u}_1$ are transverse fields already). In particular, $\mathrm{ind}(\mathbf{u}(\cdot,\, t),\, V_t) = \mathrm{ind}(\mathbf{v}(\cdot,\, t),\, V_t)$ for all t. Then one can argue, e.g. as in [121], to check that $\mathrm{ind}(\mathbf{u}_0,\, V_0) = \mathrm{ind}(\mathbf{u}_1,\, V_1)$. Here is a sketch of the argument. A standard result about transversal maps entails that the set $\psi^{-1}(Y)$ is a smooth submanifold of M, of dimension

$$\dim M - \dim E + \dim Y = (n + 1) - (2n + 1) + (n + 1) = 1,$$

hence a disjoint, finite union of smooth curves.

A closed curve in $\psi^{-1}(Y)$ cannot touch V_0 nor V_1. Indeed, assume by contradiction that there is a curve in $\psi^{-1}(Y)$ touching, say, V_0. Consider a parametrization $\gamma\colon S^1 \to V$ by a multiple of arc length. Let $\theta \in S^1$ be such that $(p,\, 0) := \gamma(\theta) \in V_0$ and denote by $\sigma\colon M \to [0,\, 1]$ the projection $(x,\, t) \mapsto t$. One has $\gamma'(\theta) \in T_{\gamma(\theta)}M \simeq T_pM_0 \oplus \mathbb{R}$. In fact, $\gamma'(\theta) \in T_pM_0$ because

$$\mathrm{d}_p\sigma\,(\gamma'(\theta)) = \frac{\mathrm{d}}{\mathrm{d}t}_{|t=\theta}\sigma(\gamma(t)) = 0,$$

as $\sigma \circ \gamma$ attains its minimum at θ. On the other hand, since $\mathbf{u}(\gamma(t)) \equiv 0$, we have

$$\mathrm{d}_p\mathbf{u}\,(\gamma'(\theta)) = \frac{\mathrm{d}}{\mathrm{d}t}_{|t=\theta}\mathbf{u}(\gamma(t)) = 0,$$

which contradicts the transversality of $\mathbf{u}_0$ because $\gamma'(\theta) \neq 0$, $\gamma'(\theta) \in T_pM_0$.

Thus, $\phi^{-1}(Y)$ is the union of smooth curves in $V \setminus (V_0 \cup V_1)$ and arcs whose endpoints are in $V_0 \cup V_1$. These endpoints are exactly the zeros of $\mathbf{u}_0$, $\mathbf{u}_1$. By considering moving tangent frames along the arcs, one sees that if an arc has both endpoints on V_0, then their contributions to the index of $\mathbf{u}_0$ are opposite and cancel each other. An analogous property holds if the arc has both the endpoints on V_1. On the other hand, the two endpoints of an arc connecting V_0 to V_1 have the same local index. Thus, summing up over all the arcs, we conclude that $\mathrm{ind}(\mathbf{u}_0,\, U_0) = \mathrm{ind}(\mathbf{u}_1,\, U_1)$. ☐

In case the domain is fixed, from this general principle we can derive the stability of the index with respect to small perturbations of the fields.

Corollary 4.3.6 (Stability). *Let $\mathbf{v}_0$, $\mathbf{v}_1$ be two continuous vector fields on $\overline{U}$, satisfying $0 \notin \mathbf{v}_0(\partial U)$, $0 \notin \mathbf{v}_1(\partial U)$. If*

$$|\mathbf{v}_0(x) - \mathbf{v}_1(x)| < |\mathbf{v}_0(x)| \qquad \textit{for all } x \in \partial U, \tag{4.3.6}$$

then $\mathrm{ind}(\mathbf{v}_0,\, U) = \mathrm{ind}(\mathbf{v}_1,\, U)$.

Proof. Set $M := X \times [0,\, 1]$, $V := U \times [0,\, 1]$ and let $\mathbf{v}\colon V \to \mathbb{R}^d$ be given by

$$\mathbf{v}(x,\, t) := (1 - t)\mathbf{v}_0(x) + t\mathbf{v}_1(x) \qquad \text{for all } (x,\, t) \in V.$$

Then $\mathbf{v}$ is a continuous function, which satisfies the hypothesis (i) of Proposition 4.3.5 because $\mathbf{v}(\cdot,\, t)$ is just a linear combination of $\mathbf{v}_0$ and $\mathbf{v}_1$. In addition, using (4.3.6) we see that

$$|(1-t)\mathbf{v}_0(x) + t\mathbf{v}_1(x)| \geq |\mathbf{v}_0(x)| - t\,|\mathbf{v}_1(x) - \mathbf{v}_0(x)| > 0$$

for all $x \in \partial U$ and all $0 \leq t \leq 1$. Hence the condition (ii) is met, so that we can invoke Proposition 4.3.5 and conclude the proof. $\square$

Corollary 4.3.6 implies that all the continuous vector fields have the same index on X. This agrees with the Poincaré-Hopf formula, which yields $\mathrm{ind}(\mathbf{v},\, X) = \chi(X)$.

Now, come back to our manifold N with boundary, and take a continuous vector field $\mathbf{v}\colon N \to \mathbb{R}^d$ such that $0 \notin \mathbf{v}(\partial N)$. The well-posedness of $\mathrm{ind}(\mathbf{v},\, N)$ in Definition 4.3.2 simply follows by taking X as the topological double of N and $U := N \setminus \partial N$.

To describe the behaviour of v at the boundary, we need to introduce another quantity. For any $x \in \partial N$, denote with $\nu(x)$ the outward unit normal to ∂N in $T_x N$. We introduce the set

$$\partial_- N[\mathbf{v}] := \{x \in \partial N \colon \mathbf{v}(x) \cdot \nu(x) < 0\}\,, \tag{4.3.7}$$

called the inward boundary, which is open in ∂N. (We simply write $\partial_- N$, when $\mathbf{v}$ is clear from the context). The tangential component $P_{\partial N}\mathbf{v}$ defines a vector field over $\partial_- N$ and, despite $0 \notin \mathbf{v}(\partial N)$, it is possible that $P_{\partial N}\mathbf{v}$ vanishes at some point. However, $P_{\partial N}\mathbf{v}$ does not vanish on $\partial(\partial_- N)$. Indeed,

$$\partial(\partial_- N) = \{x \in \partial N \colon \mathbf{v}(x) \cdot \nu(x) = 0\}\,,$$

hence if $x \in \partial(\partial_- N)$ we have $P_{\partial N}\mathbf{v}(x) = \mathbf{v}(x) \neq 0$. Thus, the following definition is well-posed.

Definition 4.3.3. Let $\mathbf{v}$ be a continuous vector field on N, such that $0 \notin \mathbf{v}(\partial N)$. We define the inward boundary index of $\mathbf{v}$ by

$$\mathrm{ind}_-(\mathbf{v},\, \partial N) := \mathrm{ind}(P_{\partial N}\mathbf{v},\, \partial_- N).$$

Notice that the inward boundary index depends only on $\mathbf{v}_{|\partial N}$. Hence, it make sense to compute it for a continuous map $\mathbf{g}$ defined only on ∂N, provided that $\mathbf{g}$ is tangent to N and vanishes nowhere. The inward boundary index is stable, with respect to small perturbations of the field.

Lemma 4.3.7. *Let $\mathbf{v}$ be a continuous fields on N satisfying $0 \notin \mathbf{v}(\partial N)$. There exists $\varepsilon_1 = \varepsilon_1(\mathbf{v}) > 0$ such that, for any other continuous vector field $\mathbf{w}$ satisfying $0 \notin \mathbf{w}(\partial N)$, if*

$$\sup_{x \in \partial N} |\mathbf{v}(x) - \mathbf{w}(x)| < \varepsilon_1$$

then $\mathrm{ind}(\mathbf{v},\, N) = \mathrm{ind}(\mathbf{w},\, N)$ *and* $\mathrm{ind}_-(\mathbf{v},\, \partial N) = \mathrm{ind}_-(\mathbf{w},\, \partial N)$.

Proof. Let $\mathbf{v}$, $\mathbf{w}$ be two continuous fields on N, satisfying $0 \notin \mathbf{v}(\partial N)$, $0 \notin \mathbf{w}(\partial N)$ and

$$\sup_{x \in \partial N} |\mathbf{v}(x) - \mathbf{w}(x)| < \varepsilon_1 := \frac{\sqrt{5}-1}{4} \min_{x \in \partial N} |\mathbf{v}(x)|. \tag{4.3.8}$$

For the sake of simplicity, set $c := \min_{\partial N} |v| > 0$. Due to (4.3.8), we deduce

$$\left| \frac{\mathbf{v}(x) \cdot \nu(x)}{|\mathbf{v}(x)|} - \frac{\mathbf{w}(x) \cdot \nu(x)}{|\mathbf{w}(x)|} \right| \leq \frac{2\varepsilon_1}{c - \varepsilon_1} \qquad \text{for all } x \in \partial N. \tag{4.3.9}$$

Indeed, for a fixed $x \in \partial N$ we suppose, e.g., that $|\mathbf{w}(x)| \leq |\mathbf{v}(x)|$. Then

$$\begin{aligned}\left|\frac{\mathbf{v}(x)\cdot\nu(x)}{|\mathbf{v}(x)|} - \frac{\mathbf{w}(x)\cdot\nu(x)}{|\mathbf{w}(x)|}\right| &\leq \left|\frac{\mathbf{v}(x)\cdot\nu(x)}{|\mathbf{v}(x)|} - \frac{\mathbf{v}(x)\cdot\nu(x)}{|\mathbf{w}(x)|}\right| + \left|\frac{\mathbf{v}(x)\cdot\nu(x)}{|\mathbf{w}(x)|} - \frac{\mathbf{w}(x)\cdot\nu(x)}{|\mathbf{w}(x)|}\right| \\ &\leq |\mathbf{v}(x)|\left(\frac{1}{|\mathbf{w}(x)|} - \frac{1}{|\mathbf{v}(x)|}\right) + \frac{|\mathbf{v}(x)-\mathbf{w}(x)|}{|\mathbf{w}(x)|} \\ &= \frac{|\mathbf{v}(x)| - |\mathbf{w}(x)|}{|\mathbf{w}(x)|} + \frac{|\mathbf{v}(x)-\mathbf{w}(x)|}{|\mathbf{w}(x)|} \\ &\leq 2\frac{|\mathbf{v}(x)-\mathbf{w}(x)|}{|\mathbf{w}(x)|},\end{aligned}$$

whence the desired inequality (4.3.9). Thus, setting

$$U_+ := \left\{x \in \partial N \colon \frac{\mathbf{w}(x)\cdot\nu(x)}{|\mathbf{w}(x)|} < \frac{2\varepsilon_1}{c-\varepsilon_1}\right\} \qquad \text{and} \qquad U_- := \left\{x \in \partial N \colon \frac{\mathbf{w}(x)\cdot\nu(x)}{|\mathbf{w}(x)|} < -\frac{2\varepsilon_1}{c-\varepsilon_1}\right\},$$

from (4.3.9) it follows that

$$U_- \subseteq \partial_- N[\mathbf{v}] \subseteq U_+ \qquad \text{and} \qquad \partial(\partial_- N[\mathbf{v}]) \subseteq \overline{U}_+ \setminus U_-.$$

Moreover, for all $x \in \overline{U}_+ \setminus U_-$ the conditions (4.3.8) and (4.3.9) imply

$$|P_{\partial N}\mathbf{w}(x)| \geq |\mathbf{w}(x)|\sqrt{1 - \frac{4\varepsilon_1^2}{(c-\varepsilon_1)^2}} \geq \sqrt{(c-\varepsilon_1)^2 - 4\varepsilon_1^2}. \tag{4.3.10}$$

By definition, ε_1 is a solution to

$$\varepsilon_1 = \sqrt{(c-\varepsilon_1)^2 - 4\varepsilon_1^2}$$

and so, in $\overline{U_+} \setminus U_-$ there holds

$$|P_{\partial N}\mathbf{v} - P_{\partial N}\mathbf{w}| \leq |\mathbf{v} - \mathbf{w}| \overset{(4.3.8)}{<} \sqrt{(c-\varepsilon_1)^2 - 4\varepsilon_1^2} \overset{(4.3.10)}{\leq} |P_{\partial N}\mathbf{w}|.$$

The condition (4.3.6) is thus satisfied, so that we can apply Corollary 4.3.6 to $P_{\partial N}\mathbf{v}$, $P_{\partial N}\mathbf{w}$, to infer

$$\mathrm{ind}_-(\mathbf{v},\, \partial N) = \mathrm{ind}(P_{\partial N}\mathbf{v},\, \partial_- N[\mathbf{v}]) = \mathrm{ind}(P_{\partial N}\mathbf{w},\, \partial_- N[\mathbf{v}]).$$

On the other hand, by (4.3.10) there is no zero of $P_{\partial N}\mathbf{w}$ in the region $\overline{U}_+ \setminus U_-$, which contains the symmetric difference between $\partial_- N[\mathbf{v}]$ and $\partial_- N[\mathbf{w}]$. Hence, Proposition 4.3.4 gives

$$\mathrm{ind}(P_{\partial N}\mathbf{w},\, \partial_- N[\mathbf{v}]) = \mathrm{ind}(P_{\partial N}\mathbf{w},\, \partial_- N[\mathbf{w}]) = \mathrm{ind}_-(\mathbf{w},\, \partial N).$$

This concludes the proof. $\square$

Morse's index formula (see Proposition 4.1.2) holds true for arbitrary continuous fields. This is actually a special case of more general Poincaré-Hopf type formula [116, Γ-existence]. For completeness, we present here a proof.

Proposition 4.3.8. *Let $\mathbf{v}$ be a continuous vector field on N, such that $0 \notin \mathbf{v}(\partial N)$. Then,*

$$\mathrm{ind}(\mathbf{v},\, N) + \mathrm{ind}_-(\mathbf{v},\, \partial N) = \chi(N).$$

Proof. We show that it is possible to approximate both $\mathbf{v}$ and $P_{\partial N}\mathbf{v}$ using the same transverse field $\mathbf{u}$. Then, the proposition will follow by applying the classical Morse's formula to $\mathbf{u}$.

Owning to the continuity of $\mathbf{v}$, we find a number $c > 0$ and a neighborhood U of ∂N in N such that

$$|\mathbf{v}(x)| \geq c \qquad \text{for all } x \in U. \tag{4.3.11}$$

Let $\varepsilon > 0$ be a small parameter, to be chosen later. We fix a smooth vector field $\tilde{\mathbf{v}}$ on N such that

$$\|\mathbf{v} - \tilde{\mathbf{v}}\|_{L^\infty(N)} \leq \varepsilon. \tag{4.3.12}$$

Then, by Theorem 4.3.2, we approximate $P_{\partial N}\tilde{\mathbf{v}}$ with a transverse vector field ξ on ∂N, such that ξ has finitely many zeros on ∂N and

$$\|P_{\partial N}\tilde{\mathbf{v}} - \xi\|_{L^\infty(\partial N)} \leq \varepsilon. \tag{4.3.13}$$

We claim that there exists a continuous vector field $\mathbf{w}$ on N, which is smooth on U, satisfies

$$\mathbf{w} = \begin{cases} \xi + \tilde{\mathbf{v}} - P_{\partial N}\tilde{\mathbf{v}} & \text{on } \partial N \\ \tilde{\mathbf{v}} & \text{on } N \setminus U \end{cases}$$

and

$$\|\mathbf{v} - \mathbf{w}\|_{L^\infty(N)} \leq C\varepsilon, \tag{4.3.14}$$

for some constant C depending only on N. (Remark that the prescribed boundary value for $\mathbf{w}$ is compatible with the condition (4.3.14), as it follows from (4.3.12) and (4.3.13)). We are giving the details of this construction in a moment, but first, we show how to conclude the proof.

By construction, $\mathbf{w}_{|\partial N}$ is a smooth function satisfying $\mathbf{v}(x) \in T_x N$ for all $x \in \partial N$. For ε small enough, (4.3.14) and Lemma 4.3.7 entail that

$$\mathrm{ind}_-(\mathbf{v},\, \partial N) = \mathrm{ind}_-(\mathbf{w},\, \partial N). \tag{4.3.15}$$

Take $\varepsilon < c/C$. Then, (4.3.11) and (4.3.14) together imply that $\mathbf{w}$ does not vanish on U. In particular, $\mathbf{w}$ is vacuously transverse on U. Using Theorem 4.3.2, we modify $\mathbf{w}$ out of U to get a transverse vector field $\mathbf{u}$, such that $\mathbf{u}_{|U} = \mathbf{w}_{|U}$. As $\mathbf{u}$ can be taken arbitrarily close to $\mathbf{w}$ in the L^∞-norm, we can assume that (4.3.4) is satisfied. Hence,

$$\mathrm{ind}(\mathbf{v},\, N) = \mathrm{ind}(\mathbf{u},\, N). \tag{4.3.16}$$

Since $\mathbf{u}$ is a transverse field, with finitely many zeros, Morse's identity applies to $\mathbf{u}$. Then, using (4.3.15) and (4.3.16), the proposition follows.

Now, let us explain how to construct the map $\mathbf{w}$. Taking a smaller U if necessary, we can assume that U is a collar of ∂N. This means, U is of the form

$$U = \{x \in N\colon\ \mathrm{dist}(x,\, \partial N) \leq \delta\}$$

for some $\delta > 0$, each point $x \in U$ has a unique nearest projection $\sigma(x) \in \partial N$, and the mapping φ given by

$$\varphi(x) := (\sigma(x),\, |x - \sigma(x)|) \qquad \text{for } x \in U$$

is a diffeomorphism $U \to \partial N \times [0,\, \delta]$. For each $x \in U$, the differential $\mathrm{d}\varphi_x$ is an isomorphism

$$T_x N \simeq T_{\sigma(x)}\partial N \oplus \mathbb{R},$$

so $T_x N$ can be decomposed into a tangential and a normal subspace, with respect to ∂N. To keep the notation simple, we assume here that $U = \partial N \times [0,\, \delta]$, and $\varphi = \mathrm{Id}_U$.

To define $\mathbf{w}$, we interpolate linearly between ξ and the tangential component of $\tilde{\mathbf{v}}$, but we leave the normal component of $\tilde{\mathbf{v}}$ unchanged. More precisely, given $x = (y,\, t) \in \partial N \times [0,\, \delta]$ we define

$$\begin{aligned} \mathbf{w}(x) &:= \left(1 - \frac{t}{\delta}\right)\xi(y) + \frac{t}{\delta} P_{\partial N}\tilde{\mathbf{v}}(x) + \tilde{\mathbf{v}}(x) - P_{\partial N}\tilde{\mathbf{v}}(x) \\ &= \left(1 - \frac{t}{\delta}\right)\Big(\xi(y) - P_{\partial N}\tilde{\mathbf{v}}(x)\Big) + \tilde{\mathbf{v}}(x) \end{aligned}$$

whereas we set

$$\mathbf{w}(x) := \tilde{\mathbf{v}}(x) \qquad \text{for } x \in N \setminus U.$$

Then $\mathbf{w}$ is of class C^1 on U, continuous on N, satisfies $\mathbf{w} = \xi + \tilde{\mathbf{v}} - P_{\partial N}\tilde{\mathbf{v}}$ on ∂N. Moreover, for $x = (y,\, t) \in U$ we have

$$\begin{aligned} |\tilde{\mathbf{v}}(x) - \mathbf{w}(x)| &\le \left(1 - \frac{t}{\delta}\right) \left|\xi(y) - P_{\partial N}\tilde{\mathbf{v}}(x)\right| \\ &\le \left(1 - \frac{t}{\delta}\right) \left(\left|\xi(y) - P_{\partial N}\tilde{\mathbf{v}}(y,0)\right| + \left|P_{\partial N}\tilde{\mathbf{v}}(y,0) - P_{\partial N}\tilde{\mathbf{v}}(y,t)\right|\right) \\ &\overset{(4.3.13)}{\le} \left(1 - \frac{t}{\delta}\right) \varepsilon + t\left(1 - \frac{t}{\delta}\right) \mathrm{Lip}_U(P_{\partial N}\tilde{\mathbf{v}}) \\ &\overset{(4.3.13)}{\le} \varepsilon + \delta C. \end{aligned}$$

By choosing δ small, and combining this inequality with (4.3.12), we deduce (4.3.14). □

4.4 The index in the VMO setting

4.4.1 Proof of Theorem 4.1.4

We have now all the necessary tools to define the index of a VMO field and prove our main results, which is the aim of this section. From now on, X will be taken to be the topological double of N, as in Section 4.2. Moreover, throughout this section we consider a function $\mathbf{g} \in \mathrm{VMO}(\partial N)$ such that

$$\mathbf{g}(x) \in T_x N \qquad \text{and} \qquad c_1 \le |\mathbf{g}(x)| \le c_2 \qquad \text{for } \mathscr{H}^{n-1}\text{-a.e. } x \in \partial N \tag{4.4.1}$$

for some constants $c_1,\, c_2 > 0$. Let $\mathbf{v}$ be a VMO vector field with trace $\mathbf{g}$, that is,

$$\mathbf{v} \in \mathrm{VMO}_{\mathbf{g}}(N), \qquad \mathbf{v}(x) \in T_x N \qquad \text{for a.e. } x \in N. \tag{4.4.2}$$

By definition of $\mathrm{VMO}_{\mathbf{g}}(N)$, the function $\mathbf{u}$ given by

$$\mathbf{u} := \begin{cases} \mathbf{v} & \text{on } N \\ \mathbf{G} & \text{on } X \setminus N, \end{cases}$$

where $\mathbf{G}$ is the extension of $\mathbf{g}$ defined in (4.2.3), is in $\mathrm{VMO}(X)$. Denote the local averages of $\mathbf{u}$ and $\mathbf{g}$ by

$$\bar{\mathbf{u}}_\varepsilon(x) := \fint_{B^X_\varepsilon(x)} \mathbf{u}(y)\, \mathrm{d}\sigma(y), \qquad \text{for } x \in X.$$

and

$$\bar{\mathbf{g}}_\varepsilon(x) := \fint_{B^{\partial N}_\varepsilon(x)} \mathbf{g}(y)\, \mathrm{d}\mathscr{H}^{n-1}(y), \qquad \text{for } x \in \partial N.$$

Consider the functions

$$\mathbf{u}_\varepsilon := P_X \bar{\mathbf{u}}_\varepsilon \qquad \text{and} \qquad \mathbf{g}_\varepsilon := P_X \bar{\mathbf{g}}_\varepsilon, \tag{4.4.3}$$

defined on X and ∂N, respectively, which are continuous and tangent to X. As we will prove in the following Lemma 4.4.1, Lemma 4.4.2, and Lemma 4.4.4, the quantities $\mathrm{ind}(\mathbf{u}_\varepsilon,\, N)$ and $\mathrm{ind}_-(\mathbf{g}_\varepsilon,\, \partial N)$ are well-defined and constant with respect to ε, for ε small enough.

Definition 4.4.1. Given $\mathbf{g} \in \mathrm{VMO}(\partial N)$ and $\mathbf{v}$ which satisfy (4.4.1)–(4.4.2), we define the index and the inward boundary index of $\mathbf{v}$ by

$$\mathrm{ind}(\mathbf{v},\, N) := \mathrm{ind}(\mathbf{u}_\varepsilon,\, N) \qquad \text{and} \qquad \mathrm{ind}_-(\mathbf{v},\, \partial N) := \mathrm{ind}_-(\mathbf{g}_\varepsilon,\, \partial N),$$

where ε is fixed arbitrarily in $(0,\, \varepsilon_0)$ and ε_0 is given by Lemma 4.4.4.

Once we have checked that the index, in the sense of Definition 4.4.1, is well-defined, Theorem 4.1.4 will follow straightforwardly from Proposition 4.3.8. However, before directing our attention to the main theorem, there are some facts which need to be checked.

The next two lemmas compare the behaviour of $\mathbf{g}_\varepsilon$ and $\mathbf{u}_{\varepsilon|\partial N}$.

Lemma 4.4.1. *For every $\delta > 0$, there exists $\varepsilon_0 \in (0,\, r_0)$ so that, for all $\varepsilon \in (0,\, \varepsilon_0)$ and all $x \in \partial N$, we have*

$$c_1 - \delta \leq |\mathbf{g}_\varepsilon(x)| \leq c_2 + \delta.$$

Lemma 4.4.2. *It holds that*

$$\lim_{\varepsilon\to 0} \sup_{x\in\partial N} |\mathbf{u}_\varepsilon(x) - \mathbf{g}_\varepsilon(x)| = 0.$$

Combining Lemmas 4.4.1 and 4.4.2, we deduce that there exist constants $\varepsilon_0, c > 0$ such that

$$|\mathbf{u}_\varepsilon(x)| \geq c, \quad |\mathbf{g}_\varepsilon(x)| \geq c \qquad \text{for all } \varepsilon \in (0,\, \varepsilon_0) \text{ and all } x \in \partial N.$$

In particular,

$$0 \notin \mathbf{u}_\varepsilon(\partial N) \qquad \text{and} \qquad 0 \notin \mathbf{g}_\varepsilon(\partial N)$$

so $\mathrm{ind}(\mathbf{u}_\varepsilon,\, N)$ and $\mathrm{ind}_-(\mathbf{g}_\varepsilon,\, \partial N)$ are well-defined, according to Definition 4.3.2 and Definition 4.3.3, for all $\varepsilon \in (0,\, \varepsilon_0)$.

Before proving Lemmas 4.4.1 and 4.4.2, we need a useful property.

Lemma 4.4.3. *It holds that*

$$\lim_{\varepsilon\to 0} \sup_{x\in X} |\mathbf{u}_\varepsilon(x) - \bar{\mathbf{u}}_\varepsilon(x)| = \lim_{\varepsilon\to 0} \sup_{x\in\partial N} |\mathbf{g}_\varepsilon(x) - \bar{\mathbf{g}}_\varepsilon(x)| = 0.$$

Proof. We present the proof for $\mathbf{u}_\varepsilon$ only, as the same argument applies to $\mathbf{g}_\varepsilon$ as well. Consider a *finite* atlas $\mathscr{A} = \{U_\alpha\}_{\alpha\in A}$ for X and, for each $\alpha \in A$, let $\nu_1^\alpha, \ldots, \nu_{d-n}^\alpha$ be a smooth moving frame for the normal bundle of X, defined on U_α (i.e., $(\nu_i^\alpha(y))_{1\leq i\leq d-n}$ is an orthonormal base for $T_yX^\perp$, for all $y \in U_\alpha$). Set

$$C_N := \max_{\substack{\alpha\in A \\ 1\leq i\leq d-n}} \|D\nu_i^\alpha\|_{L^\infty(U_\alpha)} < +\infty. \tag{4.4.4}$$

For all $\alpha \in A$ and $x \in U_\alpha$, we write

$$\mathbf{u}_\varepsilon(x) - \bar{\mathbf{u}}_\varepsilon(x) = \sum_{i=1}^{d-n} \left(\bar{\mathbf{u}}_\varepsilon(x) \cdot \nu_i^\alpha(x)\right) \nu_i^\alpha(x) \tag{4.4.5}$$

and, since $\mathbf{u}(y) \cdot \nu_i^\alpha(y) = 0$ for a.e. $y \in U_\alpha$, we have

$$\bar{\mathbf{u}}_\varepsilon(x) \cdot \nu_i^\alpha(x) = \fint_{B_\varepsilon(x)} \mathbf{u}(y) \cdot \left(\nu_i^\alpha(x) - \nu_i^\alpha(y)\right) \mathrm{d}\sigma(y).$$

Taking into account (4.4.4), we infer

$$|\bar{\mathbf{u}}_\varepsilon(x) \cdot \nu_i^\alpha(x)| \leq C_N \fint_{B_\varepsilon(x)} |\mathbf{u}(y)|\, |x - y|\, \mathrm{d}\sigma(y).$$

To bound the right-side of this inequality, we exploit the injection $\mathrm{BMO}(X) \hookrightarrow L^p(X)$, which holds true for all $1 \leq p < +\infty$, and the Hölder inequality. For a fixed p, we obtain

$$|\bar{\mathbf{u}}_\varepsilon(x) \cdot \nu_i^\alpha(x)| \leq C_N \sigma(B_\varepsilon(x))^{-1} \|x - y\|_{L^p(B_\varepsilon(x))} \|\mathbf{u}\|_{L^{p'}(X)} \leq C_{N,n,p}\, \varepsilon^{1+n/p-n} \|\mathbf{u}\|_{L^{p'}(X)}, \tag{4.4.6}$$

for some constant $C_{N,n,p}$ depending only on C_N, n and p. Whenever $p' < +\infty$, the $L^{p'}$ norm of $\mathbf{u}$ can be bounded using only the BMO norm of $\mathbf{u}$ and $⨍_X \mathbf{u}$ (with the help of [25, Lemmas A.1 and B.3]). Thus, choosing $p = p(n) > 1$ so small that $1 + n/p - n > 0$, from (4.4.5) and (4.4.6) we conclude the proof. □

Proof of Lemma 4.4.1. Setting

$$S_x := \{\mathbf{v} \in T_x N \colon c_1 \leq |\mathbf{v}| \leq c_2\}$$

we have, for all $x \in \partial N$,

$$\mathrm{dist}(\bar{\mathbf{g}}_\varepsilon(x),\, S_x) \leq ⨍_{B_\varepsilon(x)} |\bar{\mathbf{g}}_\varepsilon(x) - \mathbf{g}(y)| \,\mathrm{d}\sigma(y) + ⨍_{B_\varepsilon(x)} \mathrm{dist}(\mathbf{g}(y),\, S_x)\,\mathrm{d}\sigma(y). \tag{4.4.7}$$

The first term in the right-hand side tends to zero as $\varepsilon \to 0$, uniformly in x, due to Lemma 4.2.1. On the other hand, it holds

$$\sup_{\substack{x,\, y \in \partial N \\ \mathrm{dist}(x,\, y) \leq \varepsilon}} \ \sup_{\mathbf{v} \in S_y} \mathrm{dist}(\mathbf{v},\, S_x) \longrightarrow 0 \qquad \text{as } \varepsilon \to 0, \tag{4.4.8}$$

since N is compact and smooth up to the boundary. Formula (4.4.8) can be easily proved, e.g., by contradiction: Assume that (4.4.8) does not hold. Then, we find a number $\eta > 0$, a sequence $\{\varepsilon_k\}_{k\in\mathbb{N}}$ of positive numbers s.t. $\varepsilon_k \searrow 0$, two sequences $\{x_k\}_{k\in\mathbb{N}}$, $\{y_k\}_{k\in\mathbb{N}}$ in N and one $\{\mathbf{v}_k\}_{k\in\mathbb{N}}$ in $\mathbb{R}^d$, which satisfy

$$\mathbf{v}_k \in S_{y_k}, \qquad \mathrm{dist}(x_k,\, y_k) \leq \varepsilon_k, \qquad \mathrm{dist}(\mathbf{v}_k,\, S_{x_k}) \geq \eta.$$

By compactness of N, up to subsequences we can assume that

$$x_k \to x \in N, \qquad y_k \to y \in N, \qquad \mathbf{v}_k \to \mathbf{v} \in \mathbb{R}^d,$$

where $c_1 \leq |\mathbf{v}| \leq c_2$. Let $\nu_i, \nu_2, \ldots, \nu_{d-n}$ be a moving frame for the normal bundle of N, defined on a neighborhood of y. Passing to the limit in the condition

$$\mathbf{v}_k \cdot \nu_i(y_k) = 0 \qquad \text{for all } i$$

we find that $\mathbf{v} \in T_y N$, hence $\mathbf{v} \in S_y$. But $y = x$, because $\mathrm{dist}(x_k,\, y_k) \leq \varepsilon_k \to 0$. Thus, we have found $\mathbf{v} \in S_x$ so that $\mathrm{dist}(\mathbf{v},\, S_{x_k}) \geq \eta/2 > 0$. On the other hand, if $\varphi\colon U \subseteq N \to \mathbb{R}^n$ is a coordinate chart near x then

$$\mathbf{w}_k := \mathrm{d}\varphi^{-1}_{\varphi(x_k)}(\mathrm{d}\varphi_x \mathbf{v}), \qquad \tilde{\mathbf{w}}_k := \min\{\max\{|\mathbf{w}_k|,\, c_1\},\, c_2\} \frac{\mathbf{w}_k}{|\mathbf{w}_k|}$$

are well-defined for $k \gg 1$ and $\tilde{\mathbf{w}}_k \in S_{x_k}$, $\tilde{\mathbf{w}}_k \to \mathbf{v}$. This leads to a contradiction.

Thus, we can take advantage of (4.4.1) and (4.4.8) to estimate the second term in the right-hand side of (4.4.7). We deduce that

$$\sup_{x \in \partial N} \mathrm{dist}(\bar{\mathbf{g}}_\varepsilon(x),\, S_x) \longrightarrow 0 \qquad \text{as } \varepsilon \to 0$$

and, invoking Lemma 4.4.3, we conclude the proof. □

Proof of Lemma 4.4.2. In view of Lemma 4.4.3, proving that

$$\lim_{\varepsilon \to 0} \sup_{x \in \partial N} |\bar{\mathbf{u}}_\varepsilon(x) - \bar{\mathbf{g}}_\varepsilon(x)| = 0$$

is enough to conclude. In addition, it holds

$$|\bar{\mathbf{u}}_\varepsilon(x) - \bar{\mathbf{g}}_\varepsilon(x)| \leq \left|\bar{\mathbf{u}}_\varepsilon(x) - \bar{\mathbf{G}}_\varepsilon(x)\right| + \left|\bar{\mathbf{G}}_\varepsilon(x) - \bar{\mathbf{g}}_\varepsilon(x)\right|, \tag{4.4.9}$$

so we can study each term in the right-hand side and prove that they converge to zero as $\varepsilon \to 0$.

Let us focus on the first term. We remark that $\bar{\mathbf{u}}_\varepsilon - \bar{\mathbf{G}}_\varepsilon = \overline{(\mathbf{u} - \mathbf{G})}_\varepsilon$ and that

$$\mathbf{u} - \mathbf{G} = \begin{cases} \mathbf{v} - \mathbf{G} & \text{on } N \\ 0 & \text{on } X \setminus N. \end{cases}$$

Thus, for all $x \in \partial N$ we have (recall that $(\mathbf{u} - \mathbf{G})(y) = 0$ for almost any $y \in X \setminus N$.)

$$\begin{aligned} \frac{\sigma\left(B_\varepsilon^X(x) \setminus N\right)}{\sigma\left(B_\varepsilon^X(x)\right)} \left|\overline{(\mathbf{u} - \mathbf{G})}_\varepsilon(x)\right| &\leq \frac{1}{\sigma\left(B_\varepsilon^X(x)\right)} \int_{B_\varepsilon^X(x) \setminus N} \left|(\mathbf{u} - \mathbf{G})(y) - \overline{(\mathbf{u} - \mathbf{G})}_\varepsilon(x)\right| \, \mathrm{d}\sigma(y) \\ &\leq \fint_{B_\varepsilon^X(x)} \left|(\mathbf{u} - \mathbf{G})(y) - \overline{(\mathbf{u} - \mathbf{G})}_\varepsilon(x)\right| \, \mathrm{d}\sigma(y), \end{aligned}$$

where σ is the Riemannian measure on X. Now, assume for a while that there exist two numbers α, $\varepsilon_0 > 0$ such that

$$\frac{\sigma\left(B_\varepsilon^X(x) \setminus N\right)}{\sigma\left(B_\varepsilon^X(x)\right)} \geq \alpha \tag{4.4.10}$$

for all $x \in \partial N$ and all $\varepsilon \in (0, \varepsilon_0)$. Therefore, when $\varepsilon < \varepsilon_0$ we deduce

$$\sup_{x \in \partial N} \left|\overline{(\mathbf{u} - \mathbf{G})}_\varepsilon(x)\right| \leq \alpha^{-1} \sup_{x \in \partial N} \fint_{B_\varepsilon^X(x)} \left|(\mathbf{u} - \mathbf{G})(y) - \overline{(\mathbf{u} - \mathbf{G})}_\varepsilon(x)\right| \, \mathrm{d}\sigma(y)$$

and, since $\mathbf{u} - \mathbf{G} \in \mathrm{VMO}(X)$, the right-hand side tends to 0 as $\varepsilon \to 0$, by Lemma 4.2.1. To conclude, we have to prove the validity of (4.4.10). To this end we assume without loss of generality that N is a smooth, bounded domain in $X = \mathbb{R}^n$. For a fixed $x_0 \in \partial N$, we can locally write ∂N as the graph of a smooth function $\varphi\colon B_{r_0}(0) \subseteq \mathbb{R}^{n-1} \to \mathbb{R}$. Then, letting $L_{x_0}(x) := \varphi(x_0) + \mathrm{d}\varphi(x_0)(x - x_0)$ be the linear approximation of φ, considering the region between the graphs of φ and L_{x_0} we deduce

$$\left|\mathscr{H}^n\left(N \cap B_\varepsilon^n(x_0)\right) - \frac{1}{2}\mathscr{H}^n\left(B_\varepsilon^n(x_0)\right)\right| \leq \int_{B_\varepsilon^{n-1}(x_0)} |\varphi(x) - L_{x_0}(x)| \, \mathrm{d}x.$$

By the Taylor-Lagrange formula, we have $|\varphi(x) - L_{x_0}(x)| \leq M\,|x - x_0|^2$, for a suitable costant M controlling the hessian of φ. Thus

$$\left|\mathscr{H}^n\left(N \cap B_\varepsilon^n(x_0)\right) - \frac{1}{2}\mathscr{H}^n\left(B_\varepsilon^n(x_0)\right)\right| \leq M\omega_n\varepsilon^{n+2}\,,$$

where $\omega_n := \mathscr{H}^{n-1}(\mathbb{S}^{n-1}) = n\mathscr{H}^n(B_1^n(0))$, and

$$\left|\frac{\mathscr{H}^n\left(N \cap B_\varepsilon^n(x_0)\right)}{\mathscr{H}^n\left(B_\varepsilon^n(x_0)\right)} - \frac{1}{2}\right| \leq nM\varepsilon^2\,. \tag{4.4.11}$$

The constant M depends on φ, which is defined just locally, in a neighborhood of x_0. Nevertheless, owning to the compactness of ∂N, one needs to consider a *finite* number of functions φ only, and hence it is possible to choose a constant M which satisfies (4.4.11) for all $x_0 \in N$. Therefore, (4.4.10) follows.

Now, we have to deal with the second term in (4.4.9). We can assume, without loss of generality, that $X = \mathbb{R}^n$ and

$$N = \mathbb{R}^n_+ := \{(x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \colon x_1 \geq 0\}\,.$$

We can always reduce to this case by composing with local coordinates, with the help of a partition of the unity argument. For the sake of simplicity, denote the variable in $\mathbb{R}^n$ by $x = (t, y)$, where $t \in \mathbb{R}$ and $y \in \mathbb{R}^{n-1}$.

Call α_n the volume of the unit ball of $\mathbb{R}^n$. Using Fubini's theorem and the definition (4.2.3) of $\mathbf{G}$, for $x_0 = (0, y_0)$ and ε small enough (so that $\chi(t, y) \equiv 1$, for $|t| \le \varepsilon$) we compute

$$\begin{aligned}
\bar{\mathbf{G}}_\varepsilon(x_0) &= \frac{1}{\alpha_n \varepsilon^n} \int_{-\varepsilon}^{\varepsilon} \left(\int_{B^{n-1}(y_0,\, \sqrt{\varepsilon^2 - t^2})} \mathbf{G}(t,\, y)\, \mathrm{d}y \right) \mathrm{d}t \\
&= \frac{\alpha_{n-1}}{\alpha_n \varepsilon^n} \int_{-\varepsilon}^{\varepsilon} \left(\varepsilon^2 - t^2\right)^{\frac{n-1}{2}} \left(\fint_{B^{n-1}(y_0,\, \sqrt{\varepsilon^2 - t^2})} \mathbf{g}(y)\, \mathrm{d}y \right) \mathrm{d}t \\
&= \frac{\alpha_{n-1}}{\alpha_n \varepsilon^n} \int_{-\varepsilon}^{\varepsilon} \left(\varepsilon^2 - t^2\right)^{\frac{n-1}{2}} \bar{\mathbf{g}}_{\sqrt{\varepsilon^2 - t^2}}(y_0)\, \mathrm{d}t \\
&= \frac{\alpha_{n-1}}{\alpha_n \varepsilon^n} \int_{-1}^{1} \left(\varepsilon^2 - (\varepsilon s)^2\right)^{\frac{n-1}{2}} \bar{\mathbf{g}}_{\sqrt{\varepsilon^2 - (\varepsilon s)^2}}(y_0) \varepsilon\, \mathrm{d}s \\
&= \frac{\alpha_{n-1}}{\alpha_n} \int_{-1}^{1} \left(1 - s^2\right)^{\frac{n-1}{2}} \bar{\mathbf{g}}_{\varepsilon\sqrt{1 - s^2}}(y_0)\, \mathrm{d}s.
\end{aligned}$$

On the other hand, Fubini's theorem also implies that

$$\alpha_n = \alpha_{n-1} \int_{-1}^{1} \left(1 - t^2\right)^{\frac{n-1}{2}} \mathrm{d}t,$$

thus

$$\left|\bar{\mathbf{G}}_\varepsilon(x_0) - \bar{\mathbf{g}}_\varepsilon(x_0)\right| \le \frac{\alpha_{n-1}}{\alpha_n} \int_{-1}^{1} \left(1 - t^2\right)^{\frac{n-1}{2}} \left|\bar{\mathbf{g}}_{\varepsilon\sqrt{1-t^2}}(y_0) - \bar{\mathbf{g}}_\varepsilon(y_0)\right| \mathrm{d}t. \tag{4.4.12}$$

For all $-1 < t < 1$, since $B^{n-1}(y_0,\, \varepsilon\sqrt{1 - t^2}) \subseteq B^{n-1}(y_0,\, \sqrt{1 - t^2})$ we infer that

$$\begin{aligned}
\left|\bar{\mathbf{g}}_{\varepsilon\sqrt{1-t^2}}(y_0) - \bar{\mathbf{g}}_\varepsilon(y_0)\right| &\le \fint_{B^{n-1}(y_0,\, \varepsilon\sqrt{1-t^2})} \left|\mathbf{g}(y) - \bar{\mathbf{g}}_\varepsilon(y_0)\right| \mathrm{d}y \\
&\le \left(1 - t^2\right)^{\frac{1-n}{2}} \fint_{B^{n-1}(y_0,\, \varepsilon)} \left|\mathbf{g}(y) - \bar{\mathbf{g}}_\varepsilon(y_0)\right| \mathrm{d}y
\end{aligned}$$

and, injecting this information into (4.4.12), we deduce

$$\left|\bar{\mathbf{G}}_\varepsilon(x_0) - \bar{\mathbf{g}}_\varepsilon(x_0)\right| \le \frac{2\alpha_{n-1}}{\alpha_n} \fint_{B^{n-1}(y_0,\, \varepsilon)} \left|\mathbf{g}(y) - \bar{\mathbf{g}}_\varepsilon(y_0)\right| \mathrm{d}y.$$

Hence, applying once again Lemma 4.2.1, we conclude that the second term in the right-hand side of (4.4.9) converges to zero as $\varepsilon \to 0$, uniformly in $x \in \partial N$. $\square$

Remark 4.4.1. Setting

$$\mathrm{ind}_-(\mathbf{g},\, \partial N) := \mathrm{ind}_-(\mathbf{u}_\varepsilon,\, \partial N)$$

gives another possibility to define the inward boundary index of $\mathbf{g}$, just as natural as our Definition 4.4.1. However, thanks to Lemma 4.4.2 and to the stability of the inward boundary index (Lemma 4.3.7), we deduce that the two definitions agree.

Lemma 4.4.4. *There exists $\varepsilon_0 \in (0,\, r_0)$ so that the functions*

$$\varepsilon \mapsto \mathrm{ind}(\mathbf{u}_\varepsilon,\, N), \qquad \varepsilon \mapsto \mathrm{ind}_-(\mathbf{g}_\varepsilon,\, \partial N)$$

are constant on $(0,\, \varepsilon_0)$.

Proof. We have already remarked that $\operatorname{ind}(\mathbf{u}_\varepsilon, N)$ and $\operatorname{ind}_-(\mathbf{g}_\varepsilon, \partial N)$ are well-defined for ε small, as a consequence of Lemmas 4.4.1 and 4.4.2. Consider the functions $\mathbf{H}\colon N \times (0, \varepsilon_0) \to \mathbb{R}^d$ and $\mathbf{G}\colon \partial N \times (0, \varepsilon_0) \to \mathbb{R}^d$ given by

$$\mathbf{H}(x, \varepsilon) := \mathbf{u}_\varepsilon(x) = \operatorname{proj}_{T_x N} \bar{\mathbf{u}}_\varepsilon(x)$$

and

$$\mathbf{G}(x, \varepsilon) := \mathbf{g}_\varepsilon(x) = \operatorname{proj}_{T_x N} \bar{\mathbf{g}}_\varepsilon(x).$$

These maps are well-defined and continuous. Indeed, it follows from the dominated convergence theorem that $(x, \varepsilon) \mapsto \bar{\mathbf{u}}_\varepsilon(x)$ and $(x, \varepsilon) \mapsto \bar{\mathbf{g}}_\varepsilon(x)$ are continuous, whereas the family of projections $\operatorname{proj}_{T_x N}$ depends continuously on x. Applying Corollary 4.3.6 and Lemma 4.3.7 to $\mathbf{H}$ and $\mathbf{G}$ respectively, we conclude that $\operatorname{ind}(\mathbf{u}_\varepsilon, N)$ and $\operatorname{ind}_-(\mathbf{g}_\varepsilon, \partial N)$ are constant with respect to ε. ☐

After these preliminary lemmas, the proof of our main result, Theorem 4.1.4, is straightforward.

Proof of Theorem 4.1.4. Let $\mathbf{v}$ be given and let $\mathbf{u}_\varepsilon$ and $\mathbf{g}_\varepsilon$ be the continuous approximations of $\mathbf{v}$ and of its trace, as defined in (4.4.3). Let $\varepsilon_0 > 0$ be the constant given by Lemma 4.4.4. Up to choosing a smaller value of ε_0, owing to Lemma 4.4.1 and Lemma 4.4.2, for all $\varepsilon \in (0, \varepsilon_0)$ and all $x \in \partial N$ we have

$$|\mathbf{u}_\varepsilon(x)| \geq \frac{c_1}{2}, \quad |\mathbf{g}_\varepsilon(x)| \geq \frac{c_1}{2},$$
$$|\mathbf{u}_\varepsilon(x) - \mathbf{g}_\varepsilon(x)| < \frac{\sqrt{5}-1}{8} c_1.$$

Therefore, by Lemma 4.3.7, for all $\varepsilon \in (0, \varepsilon_0)$

$$\operatorname{ind}_-(\mathbf{u}_\varepsilon, \partial N) = \operatorname{ind}_-(\mathbf{g}_\varepsilon, \partial N). \tag{4.4.13}$$

To conclude, by Definition 4.4.1 and Proposition 4.3.8 we obtain

$$\begin{aligned}\operatorname{ind}(\mathbf{v}, N) + \operatorname{ind}_-(\mathbf{v}, \partial N) &= \operatorname{ind}(\mathbf{u}_\varepsilon, N) + \operatorname{ind}_-(\mathbf{g}_\varepsilon, \partial N) \\ &\overset{(4.4.13)}{=} \operatorname{ind}(\mathbf{u}_\varepsilon, N) + \operatorname{ind}_-(\mathbf{u}_\varepsilon, \partial N) = \chi(N),\end{aligned}$$

which proves Theorem 4.1.4. ☐

4.4.2 Proof of Proposition 4.1.5

This subsection aims at proving Proposition 4.1.5. In particular, given a boundary datum $g \in \mathrm{VMO}(\partial N)$ which satisfies (4.4.1) and the topological condition (4.1.8), we will extend it to a non vanishing VMO field defined on N.

In the following lemma, we work out the construction near the boundary. For any $r > 0$ small enough, the set

$$U_r := N \setminus N_r = \{x \in N\colon\ \operatorname{dist}(x, \partial N) < r\}$$

is a tubular neighborhood of ∂N. In particular, there exists an orientation-preserving diffeomorphism $\varphi\colon \partial N \times [0, r] \to \overline{U}_r$ such that $\operatorname{dist}(\varphi(y, s), \partial N) = s$ for any $(y, s) \in \partial N \times [0, r]$. Then, $C_r := \varphi(\partial N \times \{r\})$ is a submanifold of N, diffeomorphic to ∂N. We define the function $\bar{\mathbf{v}}\colon \overline{U}_r \to \mathbb{R}^d$ by

$$(\bar{\mathbf{v}} \circ \varphi)(y, s) := \bar{\mathbf{g}}_s(y) = \fint_{B_s^{\partial N}(y)} \mathbf{g}(z) \, \mathrm{d}\mathscr{H}^{n-1}(z) \tag{4.4.14}$$

for any $(y, s) \in \partial N \times [0, r]$, and set $\mathbf{v} := P_X \bar{\mathbf{v}}$. Thus, $\mathbf{v}$ is a tangent vector filed. Moreover, it satisfies

Lemma 4.4.5. *There exists $r > 0$ such that the following properties hold.*

(i) The set U_r is a tubular neighborhood of ∂N.

(ii) We have $\mathbf{v} \in \mathrm{VMO}(U)$, and $\mathbf{v}$ has trace $\mathbf{g}$ on ∂N (in the sense of Brezis and Nirenberg, as defined in Section 4.2).

(iii) The function $\mathbf{v}$ is continuous on $U_r \setminus \partial N$, $\mathbf{v}(x) \neq 0$ for every $x \in U_r$ and

$$\mathrm{ind}_-(\mathbf{g},\, \partial N) = \mathrm{ind}_-(\mathbf{v},\, C_r).$$

Proof. By Lemmas 4.4.1 and 4.4.4, we can pick r such that (i) holds and, in addition,

$$\frac{c_1}{2} \leq |\mathbf{g}_s| \leq 2c_2, \qquad \mathrm{ind}_-(\mathbf{g}_s,\, \partial N) = \mathrm{ind}_-(\mathbf{g},\, \partial N) \tag{4.4.15}$$

for any $0 < s \leq r$. The field $\bar{\mathbf{v}}$ is continuous on $\overline{U}_r \setminus \partial N$, due to the dominated convergence theorem, so $\mathbf{v}$ is continuous on $\overline{U}_r \setminus \partial N$. Taking a smaller r if necessary, from (4.4.15) and Lemma 4.4.3 we deduce that

$$\frac{c_1}{3} \leq |\mathbf{v}| \leq 3c_2 \qquad \text{in } \overline{U}_r. \tag{4.4.16}$$

Moreover, there holds

$$\begin{aligned} \|(\mathbf{v}\circ\varphi)(\cdot,\, r) - \mathbf{g}_r\|_{L^\infty(\partial N)} &\leq \left\| \mathrm{proj}_{T_{\varphi(\cdot,r)}X} - \mathrm{proj}_{T_{\varphi(\cdot,0)}X} \right\|_{L^\infty(\partial N)} \|\bar{\mathbf{g}}_r\|_{L^\infty(\partial N)} \\ &\overset{(4.4.1)}{\leq} C \left\| \mathrm{proj}_{T_{\varphi(\cdot,r)}X} - \mathrm{proj}_{T_{\varphi(\cdot,0)}X} \right\|_{L^\infty(\partial N)}. \end{aligned}$$

Since X is a smooth, compact manifold, $\mathrm{proj}_{T_{\varphi(\cdot,r)}X}$ converges uniformly to $\mathrm{proj}_{T_{\varphi(\cdot,0)}X}$ as $r \to 0$, so

$$\|(\mathbf{v}\circ\varphi)(\cdot,\, r) - \mathbf{g}_r\|_{L^\infty(\partial N)} \to 0 \qquad \text{as } r \to 0.$$

By the stability of the boundary index (Lemma 4.3.7), we obtain that

$$\mathrm{ind}_-((\mathbf{v}\circ\varphi)(\cdot,\, r),\, \partial N) = \mathrm{ind}_-(\mathbf{g}_r,\, \partial N)$$

if r is small enough. On the other hand, the index and the boundary index are invariant by composition with a diffeomorphism. (For smooth, transverse vector fields, this follows by Formula (4.3.1); for arbitrary continuous fields $\mathbf{v}$ satisfying $0 \notin \mathbf{v}(\partial N)$, one argues by density.) Therefore, we conclude that

$$\mathrm{ind}_-(\mathbf{v},\, C_r) = \mathrm{ind}_-(\mathbf{g}_r,\, \partial N) \overset{(4.4.15)}{=} \mathrm{ind}_-(\mathbf{g},\, \partial N),$$

and (iii) holds true.

We only need to check that $\mathbf{v} \in \mathrm{VMO}(U_r)$, with trace $\mathbf{g}$ on ∂N; this is equivalent to proving that the map

$$\mathbf{u} := \begin{cases} \mathbf{v} & \text{on } U_r \\ \mathbf{G} & \text{on } X \setminus N \end{cases}$$

belongs to $\mathrm{VMO}(U_r \cup (X \setminus N))$. (Here $\mathbf{G} \in \mathrm{VMO}(X)$ denotes the standard extension of $\mathbf{g}$, as defined in (4.2.3).) By [26, Theorem 1, Eq. (1.2)], this is also equivalent to

$$\sup_{x \in W_{r-2\varepsilon}} I_\varepsilon(\mathbf{u},\, x) \to 0 \qquad \text{as } \varepsilon \to 0, \tag{4.4.17}$$

where we have set

$$I_\varepsilon(\mathbf{u},\, x) := \fint_{B^X_\varepsilon(x)} \fint_{B^X_\varepsilon(x)} |\mathbf{u}(y) - \mathbf{u}(z)| \, \mathrm{d}\sigma(y) \, \mathrm{d}\sigma(z)$$

and $W_s := U_s \cup (X \setminus N)$, for any s. Thanks to [25, Lemma 7], we know that $\bar{\mathbf{v}} \in \mathrm{VMO}(U_r)$ has trace $\mathbf{g}$ at the boundary, that is the map

$$\bar{\mathbf{u}} := \begin{cases} \bar{\mathbf{v}} & \text{on } U_r \\ \mathbf{G} & \text{on } X \setminus N \end{cases}$$

belongs to $\mathrm{VMO}(W_r)$. This yields

$$\sup_{x \in W_{r-2\varepsilon}} I_\varepsilon(\bar{\mathbf{u}},\, x) \to 0 \qquad \text{as } \varepsilon \to 0 \tag{4.4.18}$$

(again by [26, Theorem 1]). For a fixed $0 < s < r$ and $0 < \varepsilon < (r-s)/2$, there holds

$$\sup_{x \in W_{r-2\varepsilon}} I_\varepsilon(\mathbf{u},\, x) \leq \max \left\{ \sup_{x \in W_{s-\varepsilon}} I_\varepsilon(\bar{\mathbf{u}},\, x) + 2 \left\| \bar{\mathbf{u}} - \mathbf{u} \right\|_{L^\infty(U_s)},\ \sup_{x \in U_{r-2\varepsilon} \setminus U_{s-\varepsilon}} I_\varepsilon(\mathbf{u},\, x) \right\}.$$

We take the upper limit as $\varepsilon \to 0$. Using (4.4.18) and the fact that $\mathbf{u}$ is continuous on $N \setminus \partial N$, we deduce

$$\limsup_{\varepsilon \to 0} \sup_{x \in W_{r-2\varepsilon}} I_\varepsilon(\mathbf{u},\, x) \leq 2 \left\| \bar{\mathbf{u}} - \mathbf{u} \right\|_{L^\infty(U_s)}.$$

Now, we let $s \to 0$. By applying Lemma 4.4.3, we conclude that (4.4.17) holds, so $\mathbf{u} \in \mathrm{VMO}(W_r)$. $\square$

We can finally give the proof of Proposition 4.1.5.

Proof of Proposition 4.1.5. Since a field $\mathbf{v} \in \mathrm{VMO}_{\mathbf{g}}(N)$ satisfying (4.1.4) has $\mathrm{ind}(\mathbf{v},\, N) = 0$, Theorem 4.1.4 directly implies (4.1.8). In order to prove the converse implication, let a field $\mathbf{g} \in \mathrm{VMO}(\partial N)$ be given, such that (4.1.5) and (4.1.8) hold. Let $\mathbf{v}\colon U_r \to \mathbb{R}^d$ be the field defined by (4.4.14), where $r > 0$ is given by Lemma 4.4.5. Let $\mathbf{V}\colon N \setminus U_r \to \mathbb{R}^d$ be any continuous field such that $\mathbf{V} = \mathbf{v}$ on $C_r = \partial(N \setminus U_r)$. (For instance, one can take as $\mathbf{V}$ the standard extension of $\mathbf{v}_{|C_r}$, as defined by (4.2.3).) As $0 \notin \mathbf{V}(C_r)$, by the Transversality Theorem 4.3.2 there exists a smooth tangent vector field $\mathbf{F}$ on X such that $\mathbf{F}$ has finitely many zeros in $N \setminus U_r$, $\mathbf{F}_{|C_r} = \mathbf{v}_{|C_r}$ and, by stability (Corollary 4.3.6) and by Theorem 4.1.4, that

$$\begin{aligned} \mathrm{ind}(\mathbf{F},\, N \setminus U_r) &= \mathrm{ind}(\mathbf{V},\, N \setminus U_r) = \chi(N) - \mathrm{ind}_-(\mathbf{v},\, C_r) \\ &\overset{(iii)}{=} \chi(N) - \mathrm{ind}_-(\mathbf{g},\, \partial N) \overset{(4.1.8)}{=} 0. \end{aligned}$$

Let $\tilde{\mathbf{F}}$ be defined by $\tilde{\mathbf{F}} := \mathbf{v}$ on U_r and $\tilde{\mathbf{F}} := \mathbf{F}$ on $N \setminus U_r$. The field $\tilde{\mathbf{F}}$ is continuous on the interior of N, belongs to $\mathrm{VMO}_{\mathbf{g}}(N)$ and satisfies $\mathbf{F}(x) \neq 0$ for any $x \in U_r$, by Lemma 4.4.5. Assume for the moment that $\mathbf{F}(x) \neq 0$ for all $x \in N \setminus U_r$, and set

$$A_1 := \{x \in N\colon |\tilde{\mathbf{F}}(x)| < c_1\}, \qquad A_2 := \{x \in N\colon |\tilde{\mathbf{F}}(x)| > c_2\}.$$

Then, the field defined by

$$\mathbf{V}(x) := \begin{cases} c_i |\tilde{\mathbf{F}}(x)|^{-1} \tilde{\mathbf{F}}(x) & \text{if } x \in A_i,\ i = 1, 2, \\ \tilde{\mathbf{F}}(x) & \text{otherwise.} \end{cases}$$

belongs to $\mathrm{VMO}_{\mathbf{g}}(N)$ and satisfies (4.1.4).

To conclude, we note that there is a standard technique to modify a continuous field $\mathbf{u}$ such that

$$0 \notin \mathbf{u}(\partial N), \qquad \mathrm{ind}(\mathbf{u},\, N) = 0, \qquad \text{and} \qquad \#\{x \in N\colon \mathbf{u}(x) = 0\} < +\infty$$

into a continuous field $\tilde{\mathbf{u}}$ such that $|\tilde{\mathbf{u}}| > 0$ and $\tilde{\mathbf{u}} = \mathbf{u}$ on ∂N. (We will apply this technique to $\mathbf{u} = \mathbf{F}$ over $N \setminus U_r$.) We sketch here the idea. First, up to a continuous transformation, we can assume that all the zeros are contained in one coordinate neighborhood U, with chart $\phi\colon U \subseteq N \to D \subseteq \mathbb{R}^n$, so we can reduce to study the vector field in coordinates: let $D := B_1(0)$, $D_{1/2} := B_{1/2}(0)$, assume that $\mathbf{u}\colon D \to \mathbb{R}^n$ and $|\mathbf{u}| > 0$ in $D \setminus D_{1/2}$. Then,

$$0 = \operatorname{ind}(\mathbf{u},\, D) = \deg\left(\frac{\mathbf{u}}{|\mathbf{u}|},\, \partial D,\, \mathbb{S}^{n-1}\right).$$

and there exists a continuous field $\psi\colon D \to \mathbb{S}^{n-1}$ such that $\psi_{|\partial D} = |\mathbf{u}|^{-1}\mathbf{u}$. Define

$$\tilde{\psi}(x) := \begin{cases} \psi(x) & \text{if } x \in D_{1/2} \\ \psi(x)(2\operatorname{dist}(x, \partial D) + (1 - 2\operatorname{dist}(x, \partial D)|\mathbf{u}(x)|)) & \text{if } x \in D \setminus D_{1/2}, \end{cases}$$

so that $\tilde{\psi}(x)$ is continuous on D, nowhere zero, and it agrees with $\mathbf{u}$ on ∂D. To conclude, the field

$$\tilde{\mathbf{u}}(x) := \begin{cases} \mathbf{u}(x) & \text{if } x \in N \setminus U \\ \phi^* \tilde{\psi}(x) & \text{if } x \in U \end{cases}$$

is continuous and nowhere zero on N. Here $\phi^*\tilde{\psi}(x) := \mathrm{d}\phi^{-1}_{\phi(x)}\tilde{\psi}(\phi(x))$ denotes the usual pullback of $\tilde{\psi}$ via ϕ. □

Corollary 4.4.6. *Let $1 < p < +\infty$, and let $\mathbf{g} \in W^{1-1/p,p}(\partial N)$ be a vector field satisfying* (4.1.5) *and* (4.1.8). *Then, there exists $\mathbf{v} \in W^{1,p}(N)$ which satisfies* (4.1.4) *and has trace $\mathbf{g}$ at the boundary.*

Proof. The extension $V \in \mathrm{VMO}_{\mathbf{g}}(N)$ we have constructed in the previous proof is actually continuous in the interior of N and smooth in $N \setminus U_r$. Therefore, the result will be proved if we show that the field $\mathbf{v}$, defined by (4.4.14), belongs to $W^{1,p}(U_r)$ when $\mathbf{g} \in W^{1-1/p}(\partial N)$. By using a partition of unity and composing with local diffeomorphisms, we can assume with no loss of generality that $U_r = \Sigma_r \times [0, \varepsilon]$, where $\Sigma_r := [\varepsilon,\, 1-\varepsilon]^{n-1}$ and $\mathbb{R}^{n-1}$ is endowed with the norm $\|x\| := \max_i |x_i|$. Then, Formula (4.4.14) reduces to

$$\mathbf{v}(x) = \frac{1}{(2x_n)^{n-1}} \int_{x_1 - x_n}^{x_1 + x_n} \mathrm{d}\xi_n \ldots \int_{x_{n-1} - x_n}^{x_{n-1} + x_n} \mathrm{d}\xi_{n-1}\, \mathbf{g}(\xi_1,\, \ldots,\, \xi_{n-1}). \tag{4.4.19}$$

In his paper [50], Gagliardo used functions of this form [5] to prove the existence of a right inverse for the trace operator $W^{1,p}(\Omega) \to W^{1-1/p,p}(\partial\Omega)$. More precisely, he proved that

$$\|\mathbf{v}\|_{W^{1,p}(U_r)} \leq C\, \|\mathbf{g}\|_{W^{1-1/p,p}(\Sigma_0)}\, .$$

This shows that $\mathbf{v} \in W^{1,p}(U_r)$ as soon as $\mathbf{g} \in W^{1-1/p,p}(\Sigma_0)$, and concludes the proof. □

Remark 4.4.2. In our main results, Theorem 4.1.4 and Proposition 4.1.5, the boundary datum $\mathbf{g}$ and the field $\mathbf{v}$ are assumed to satisfy inequalities such as

$$c_1 \leq |\mathbf{g}(x)| \leq c_2 \qquad \text{for a.e. } x \text{ and positive constants } c_1, c_2$$

(see (4.4.1), (4.4.2)). The lower bound is the natural generalization of the condition $\mathbf{g}(x) \neq 0$, which makes no sense as the field $\mathbf{g}$ is not defined pointwise everywhere. On the other hand, the upper bound is a technical assumption, which is used only in the proof of Lemma 4.4.1 to control the last term in (4.4.7). For our purposes, this assumption is not restrictive, since we are interested mainly in unit vector fields. However, after our results were announced, Van Schaftingen remarked that the upper bound on $\mathbf{g}$ is unnecessary. For the sake of completeness, we state here Van Schaftingen's alternative argument, in the form of an independent lemma.

5. Actually, Gagliardo considered a function of the form

$$\mathbf{v}_*(x) = \frac{1}{x_n^{n-1}} \int_{x_1}^{x_1 + x_n} \mathrm{d}\xi_n \ldots \int_{x_{n-1}}^{x_{n-1} + x_n} \mathrm{d}\xi_{n-1}\, \mathbf{g}(\xi_1,\, \ldots,\, \xi_{n-1}),$$

but his computations can be adapted straightforward way to $\mathbf{v}$ defined by (4.4.19).

Lemma 4.4.7. *Let* $\mathbf{g} \in \mathrm{VMO}(\partial N)$ *be such that*

$$\mathbf{g}(x) \in T_x N \qquad \text{and} \qquad |\mathbf{g}(x)| \geq c, \tag{4.4.20}$$

for $\mathscr{H}^{n-1}$*-a.e.* $x \in \partial N$ *and some constant* $c > 0$*. For every* $\delta > 0$*, there exists* $\varepsilon_0 \in (0, r_0)$ *such that, for all* $\varepsilon \in (0, \varepsilon_0)$ *and all* $x \in \partial N$*, there holds*

$$|\mathbf{g}_\varepsilon(x)| \geq c - \delta.$$

Proof. For each $x \in \partial N$, define the set

$$\tilde{S}_x := \{\mathbf{v} \in T_x N \colon \ |\mathbf{v}| \geq c_1\},$$

so that $\mathbf{g}(x) \in \tilde{S}_x$ for a.e. x due to (4.4.20). Note that the sets $\tilde{S}_x$ do *not* satisfy the condition (4.4.8) (two vectors $\mathbf{v}_1 \in \tilde{S}_x$ and $\mathbf{v}_2 \in \tilde{S}_y$ with $|\mathbf{v}_1| \gg 1$, $|\mathbf{v}_2| \gg 1$ may be far from each other even if y is very close to x, due to the curvature of the manifold). Nevertheless, as in (4.4.7), we have

$$\mathrm{dist}(\bar{\mathbf{g}}_\varepsilon(x), \tilde{S}_x) \leq \fint_{B_\varepsilon^{\partial N}(x)} |\bar{\mathbf{g}}_\varepsilon(x) - \mathbf{g}(y)| \, \mathrm{d}\sigma(y) + \fint_{B_\varepsilon^{\partial N}(x)} \mathrm{dist}(\mathbf{g}(y), T_x N) \, \mathrm{d}\sigma(y) \tag{4.4.21}$$

and the first term converges to zeros uniformly in x as $\varepsilon \to 0$, due to Lemma 4.2.1. To control the second term, we use the following fact: if $x, y \in N$ are close enough to each other and $\mathbf{v} \in T_y N$, then

$$\mathrm{dist}(\mathbf{v}, T_x N) \leq C \, |\mathbf{v}| \, \mathrm{dist}(x, y). \tag{4.4.22}$$

We postpone the proof of this claim. With the help of (4.4.22) and Jensen inequality, we obtain

$$\begin{aligned}
\fint_{B_\varepsilon^{\partial N}(x)} \mathrm{dist}(\mathbf{g}(y), T_x N) \, \mathrm{d}\sigma(y) &\leq C\varepsilon \fint_{B_\varepsilon^{\partial N}(x)} |\mathbf{g}(y)| \, \mathrm{d}\sigma(y) \\
&\leq C\varepsilon \left(\fint_{B_\varepsilon^{\partial N}(x)} |\mathbf{g}(y)|^n \, \mathrm{d}\sigma(y) \right)^{1/n} \\
&= C\varepsilon^{1 - \frac{n-1}{n}} \left(\int_{B_\varepsilon^{\partial N}(x)} |\mathbf{g}(y)|^n \, \mathrm{d}\sigma(y) \right)^{1/n} \\
&\leq C\varepsilon^{1/n} \, \|\mathbf{g}\|_{\mathrm{VMO}(\partial N)} \to 0.
\end{aligned}$$

The last inequality follows by the continuous embedding $\mathrm{VMO}(\partial N) \hookrightarrow L^n(\partial N)$. Therefore, it only remains to prove (4.4.22). We fix $x, y \in N$ and $\mathbf{v} \in N$, and we consider a coordinate chart

$$\varphi \colon U \subseteq N \to \mathbb{R}^n$$

defined in a neighborhood of x and y. Set $x_0 := \varphi(x)$, $y_0 = \varphi(y)$, $\mathbf{v}_0 := \mathrm{d}\varphi_y(\mathbf{v})$ and $\mathbf{u}_0 := \mathbf{v}_0/|\mathbf{v}_0|$. We have $\mathrm{d}\varphi_{y_0}^{-1}(\mathbf{v}_0) = \mathbf{v}$ and $\mathrm{d}\varphi_{x_0}^{-1}(\mathbf{v}_0) \in T_x N$, so

$$\mathrm{dist}(\mathbf{v}, T_x N) \leq \left| \mathrm{d}\varphi_{y_0}^{-1}(\mathbf{v}_0) - \mathrm{d}\varphi_{x_0}^{-1}(\mathbf{v}_0) \right| = |\mathbf{v}_0| \left| \mathrm{d}\varphi_{y_0}^{-1}(\mathbf{u}_0) - \mathrm{d}\varphi_{x_0}^{-1}(\mathbf{u}_0) \right|.$$

By applying Lagrange's mean value theorem to the function $z \mapsto \mathrm{d}\varphi_z^{-1}(\mathbf{u}_0) = \partial \varphi^{-1}/\partial \mathbf{u}_0(z)$, we deduce that

$$\left| \mathrm{d}\varphi_{y_0}^{-1}(\mathbf{u}_0) - \mathrm{d}\varphi_{x_0}^{-1}(\mathbf{u}_0) \right| \leq C \, |y_0 - x_0|,$$

for some constant C which bounds from above the norm of $\mathrm{D}^2\varphi^{-1}$. Because of the Lipschitz continuity of φ, we infer that

$$|\mathbf{v}_0| \left| \mathrm{d}\varphi_{y_0}^{-1}(\mathbf{u}_0) - \mathrm{d}\varphi_{x_0}^{-1}(\mathbf{u}_0) \right| \leq C \, |\mathbf{v}_0| \, |y_0 - x_0| \leq C \, |\mathbf{v}| \, \mathrm{dist}(x, y),$$

whence (4.4.22) follows. Since ∂N is compact, one has to consider a finite number of local charts only, so the constant C can be chosen independently of φ. $\square$

4.5 An application: Q tensor fields and line fields.

In the mathematical modelling of Liquid Crystals two different theories are eminent. In the Frank-Oseen theory the molecules are represented by the unit vector field $\mathbf{n}$ which appears in the energy (4.1.1). The main drawback of this approach is to neglect the natural head-to-tail symmetry of the crystals. The theory of Landau-de Gennes takes this symmetry into account by introducing a tensor-valued field, called *Q-tensor*, to which is associated a scalar parameter s that represents the local average ordered/disordered state of the molecules. In the particular, but physically relevant, case when the order parameter is a positive constant, there is a bijection between Q-tensors and line fields. The differences between the vector-based and the line field-based theory have been studied in [10], in two- and three-dimensional Euclidean domains. In this Section we have two aims: firstly we apply the results obtained in Section 4.4 to line fields on a compact surface, obtaining the VMO-analogue of Poincaré-Kneiser Theorem (see Theorem 4.5.2 below); secondly we show how the question of orienting a line field, studied in [10], has generally a negative answer on a compact surface. As it happens for liquid crystals in Euclidean domains, the elastic part of the Landau-de Gennes energy for nematic shells is, at least in some simplified situations, proportional to a Dirichlet type energy. See on this regard [80] and [110]. Therefore, owing to the embedding of Sobolev spaces in VMO spaces, (4.1.3), Proposition 4.5.3 establishes a relation between the existence of finite energy Q-tensors with strictly positive order parameter and the topology of the underlying surface, thus extending our application scope from the Frank-Oseen theory to the (constrained) Landau-de Gennes one, for uniaxial nematic shells.

4.5.1 Q-tensors and line fields

Nematic shells are the datum of a compact, connected and without boundary surface $N \subseteq \mathbb{R}^3$ coated with a thin film of rod-shaped, head-to-tail symmetric particles of nematic liquid crystal. At a given point $x \in N$, the local configuration is represented by a probability measure μ_x on the unit circle S_x in T_xN. More precisely, for each Borel set $A \subseteq S_x$, $\mu_x(A)$ is the probability of finding a particle at x, with direction contained in A. To account for the symmetry of the particles, we require

$$\mu_x(A) = \mu_x(-A) \tag{4.5.1}$$

for each Borel set $A \subseteq S_x$. Due to this constraint, the first-order momentum of μ_x vanishes. Hence, we are naturally led to consider the second-order momentum

$$Q = \sqrt{2} \int_{S_x} \left(\mathbf{p}^{\otimes 2} - \frac{1}{2} P_x \right) \mathrm{d}\mu_x(\mathbf{p}), \tag{4.5.2}$$

where $(\mathbf{p}^{\otimes 2})_{ij} := \mathbf{p}^i \mathbf{p}^j$ and P_x denotes the orthogonal projection on T_xN. Note that Q has been suitably renormalized, so that $Q = 0$ when μ_x is the uniform measure, and $|Q| = 1$ when μ_x is a Dirac measure concentrated on one direction (see (4.5.6) and (4.5.7)). This formula defines a real 3×3 symmetric and traceless matrix called *Q-tensor*. As we are interested in fields on surfaces, we replaced the usual three-dimensional renormalization term $-\frac{1}{3}\,\mathrm{Id}$ by $-\frac{1}{2}P_x$ (see, e.g., [80]). Once we have fixed an orientation on N, we let γ denote the Gauss map. By definition (4.5.2), $Q\gamma(x) = 0$, which translates the intuitive fact that the probability of finding a particle in the normal direction of the surface is zero. We call this type of anchoring a *degenerate (tangent) anchoring* (see [110]).

For any $x \in N$ we define the class of "admissible tensors" at x as

$$\mathbf{Q}_x := \{Q \in \mathbf{S}_0 \colon Q\gamma(x) = 0\}, \tag{4.5.3}$$

where $\mathbf{S}_0$ is the space of 3×3 real, symmetric, and traceless matrices, endowed with the scalar product $Q \cdot P = \sum_{ij} Q_{ij} P_{ij}$. It is clear from the definition that $\mathbf{Q}_x$ is a linear subspace of $\mathbf{S}_0$ of dimension 2 (this can be easily checked, e.g., by proving that the map $\mathbf{S}_0 \to \mathbb{R}^3$ given by $Q \mapsto Q\gamma(x)$ is surjective). Moreover, $\mathbf{Q}_x$ varies smoothly with x.

Lemma 4.5.1. *The set*
$$\mathbf{Q} := \coprod_{x\in N} \mathbf{Q}_x,$$
equipped with the natural projection $(x, Q) \mapsto x$*, is a smooth vector bundle on* N*.*

Proof. Consider a smooth orthonormal frame $(\mathbf{n}, \mathbf{m}, \gamma)$ defined on a coordinate neighborhood of N, where $(\mathbf{n}, \mathbf{m})$ is a basis for the tangent bundle of N. With straightforward computations, one can see that the matrices
$$X_{ij} := n_i n_j - m_i m_j, \qquad Y_{ij} := n_i m_j + m_i n_j,$$
$$E_{ij} := \gamma_i\gamma_j - \frac{1}{3}\delta_{ij}, \qquad F_{ij} := n_i\gamma_j + \gamma_i n_j, \qquad G_{ij} := m_i\gamma_j + \gamma_i m_j$$
define an orthogonal frame for $\mathbf{S}_0$. Moreover, $(X(x), Y(x))$ is a basis for $\mathbf{Q}_x$, at each point x (see, e.g., [73] for a use of this basis with a particular choice for $(\mathbf{n}, \mathbf{m}, \gamma)$). The lemma follows easily. ☐

We can now analyze the special structure of the matrices in $\mathbf{Q}_x$. Fix $Q \in \mathbf{Q}_x$, from (4.5.3) it follows that $\gamma(x)$ is an eigenvector of Q, corresponding to the zero eigenvalue. Since Q is symmetric and traceless, there exists an orthonormal basis $(\mathbf{n}, \mathbf{m})$ of T_xN, whose elements are eigenvectors of Q, and the corresponding eigenvalues are opposite. Thus, denoting by $\mathbf{n}$ the eigenvector corresponding to the positive eigenvalue, Q can be written in the form

$$Q = \frac{s}{2}\left(\mathbf{n}^{\otimes 2} - \mathbf{m}^{\otimes 2}\right) \tag{4.5.4}$$

for some $s \geq 0$ (If $s = 0$, then $Q = 0$ and any choice of $\mathbf{n}$ is allowed). Using the identity $\mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2} = P_x$, we conclude that for each $Q \in \mathbf{Q}_x$ there exist a number $s \geq 0$ and a unit vector $\mathbf{n} \in T_xN$ such that

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{2}P_x\right). \tag{4.5.5}$$

The number s, called the order parameter, is uniquely determined, and from (4.5.4) we obtain

$$|Q|^2 = Q\cdot Q = \frac{s^2}{4}\left(\mathbf{n}^{\otimes 2} - \mathbf{m}^{\otimes 2}\right)\cdot\left(\mathbf{n}^{\otimes 2} - \mathbf{m}^{\otimes 2}\right) = \frac{s^2}{4}\left(\mathbf{n}^{\otimes 2}\cdot\mathbf{n}^{\otimes 2} + \mathbf{m}^{\otimes 2}\cdot\mathbf{m}^{\otimes 2}\right) = \frac{s^2}{2}. \tag{4.5.6}$$

When $Q \neq 0$, $\mathbf{n}$ is also uniquely determined, up to a sign. Thus, each $Q \in \mathbf{Q}_x \setminus \{0\}$ identifies a positive number and a (unoriented) direction in T_xN, that is, a *line field*.

A *line field* on N (also called *1-distribution*) is an assignment of a (non zero) tangent direction — but not an orientation — to each point of the submanifold N. More precisely, following [134, Chapter 6] a line field L is a function that assigns to each point x of a manifold N a one-dimensional subspace $L(x) \subseteq T_xN$. Then L is spanned by a vector field *locally*; that is, we can choose a vector field $\mathbf{v}$ such that $0 \neq \mathbf{v}(x) \in L(x)$ for all x in some neighborhood of x. We say that L is a smooth (continuous) 1-distribution if the vector field $\mathbf{v}$ can be chosen to be smooth (continuous) in a neighborhood of each point.

Conversely, to a given line $\ell \subseteq T_xN$ generated by a unit vector $\xi \in T_xN$ it is possible to associate the measure $\mu_x := \frac{1}{2}\delta_\xi + \frac{1}{2}\delta_{-\xi}$ and thus by (4.5.2) the direction ξ corresponds to

$$Q = \sqrt{2}\left(\xi^{\otimes 2} - \frac{1}{2}P_x\right), \tag{4.5.7}$$

which is a unit Q-tensor. The reason for associating to the direction ξ the measure $\mu_x = \frac{1}{2}\delta_\xi + \frac{1}{2}\delta_{-\xi}$, instead of simply δ_ξ, is to be found in the head-to-tail symmetry of the molecules expressed by (4.5.1). Thus, line fields on N can be identified with sections of the bundle $\mathbf{Q}$, having modulus one.

In the following, we relax the condition $|Q| = 1$, by requiring $|Q|$ to be bounded and uniformly positive.

4.5.2 Existence of VMO line fields

In what follows, we assume that $N \subseteq \mathbb{R}^3$ is a smooth, compact, connected surface, without boundary. Based on Proposition 4.1.1 and on the results of Section 4.4, in Proposition 4.5.3 we prove that the existence of a VMO line field is subject to the same topological obstruction that holds for continuous vector fields. If we restrict to the continuous setting, the following result is classical (see, e.g., [65, Theorem 2.4.6, p. 24])

Theorem 4.5.2 (Poincaré-Kneiser)**.** *Let N be a compact, connected submanifold of $\mathbb{R}^{n+1}$. Then a continuous line field exists if and only if $\chi(N) = 0$.*

Definition 4.5.1. A VMO line field on N is a map $Q \in \mathrm{VMO}(N, \mathbf{S}_0)$, such that

$$Q(x) \in \mathbf{Q}_x \qquad \text{and} \qquad c_1 \leq |Q(x)| \leq c_2 \tag{4.5.8}$$

for some constants $c_1, c_2 > 0$ and $\mathscr{H}^2$-a.e. $x \in N$.

The condition $Q \in \mathrm{VMO}(N, \mathbf{S}_0)$ makes perfectly sense, because $\mathbf{S}_0 \simeq \mathbb{R}^5$ is a finite-dimensional linear space.

Proposition 4.5.3. *If a* VMO *line field on N exists, then $\chi(N) = 0$, that is, N has genus* 1*.*

Proof. The proof is based on the arguments of Section 4.4, with straightforward adaptations. We approximate Q with a family of continuos functions, by setting

$$\bar{Q}_\varepsilon(x) := \fint_{B^n_\varepsilon(x)} Q(y)\, \mathrm{d}\sigma(y)$$

for each $x \in N$ and $\varepsilon \in (0, r_0)$. Then, we define

$$Q_\varepsilon(x) := \mathrm{proj}_{\mathbf{Q}_x} \bar{Q}_\varepsilon(x) \qquad \text{for } x \in N.$$

The functions Q_ε are continuous, since the Q_x's vary smoothly (see Lemma 4.5.1). Owing to (4.5.8), and arguing as in Lemma 4.4.1, it can be proved that

$$\frac{c_1}{2} \leq |Q_\varepsilon(x)| \leq 2c_2$$

for all $x \in N$ and ε small enough. In view of formula (4.5.5), each Q_ε induces a continuous line field on N. In fact, the continuity of Q_ε gives the continuity of $|Q_\varepsilon|$. Consequently, we have that s is a continuous function, thanks to (4.5.6). On the other hand, the representation formula (4.5.5) gives that

$$\mathbf{n}^{\otimes 2}(x) = \frac{Q(x)}{s(x)} + \frac{1}{2} P_x,$$

which implies the continuity of $\mathbf{n}^{\otimes 2}$ thanks to the assumed strict positivity of s and thanks to the continuity of the projection operator. The tensor $\mathbf{n}^{\otimes 2}$ is the line field we were looking for. Thus, by Theorem 4.5.2, it must be $\chi(N) = 0$. $\square$

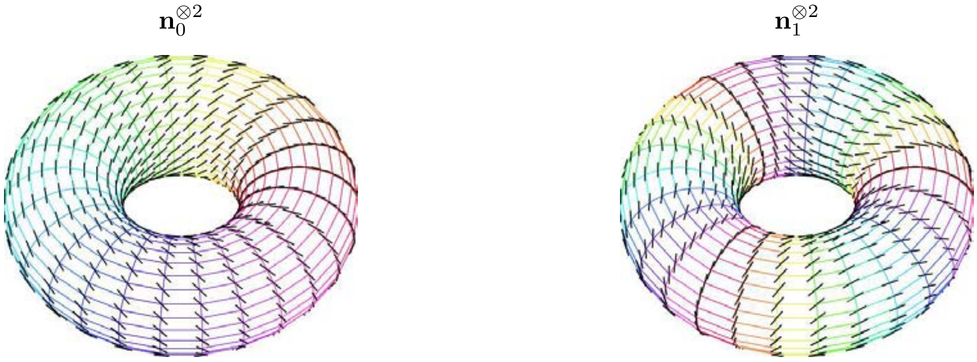


Figure 4.2: The case of an axisymmetric torus, with radii $R = 2$, $r = 1$, parametrized by $X\colon (\theta,\, \phi) \mapsto ((2+\cos\theta)\cos\phi,\, (2+\cos\theta)\sin\phi,\, \sin\theta)$, on $[0,\, 2\pi) \times [0, 2\pi)$. Let $\mathbf{e}_\theta := |\partial_\theta X|^{-1}\partial_\theta X$, $\mathbf{e}_\phi := |\partial_\phi X|^{-1}\partial_\phi X$. We give a schematic representation of the two line fields defined via $\mathbf{n}_i(\theta,\, \phi) := \cos\left((i+1/2)\phi\right)\mathbf{e}_\theta + \sin\left((i+1/2)\phi\right)\mathbf{e}_\phi$ for $i \in \{0,\, 1\}$.

4.5.3 Orientability of line fields

A typical problem in the study of line fields is to understand in which circumstances a Q-tensor can be described in terms of a vector, that is when, given a tensor field Q with a specified regularity, one can find a unit vector field $\mathbf{n}$ with the same regularity, such that (in three dimensions)

$$Q = s\left(\mathbf{n}^{\otimes 2} - \frac{1}{3}\,\mathrm{Id}\right) \tag{4.5.9}$$

for some positive constant s. In other words, we are trying to prescribe an orientation for the Q-tensor without creating artificial discontinuities in the vector $\mathbf{n}$. If for a given tensor Q we can find a vector $\mathbf{n}$ for which the representation (4.5.9) holds, we say that Q is *orientable*, otherwise *non-orientable*. The problem of the orientability of a Q-tensor has been addressed and solved by Ball and Zarnescu in [10], in the case of two- and three-dimensional Euclidean domains. They showed that the conditions for orienting a given tensor field are of topological as well as of analytical nature. Precisely, they require a Sobolev-type regularity, i.e. $Q \in W^{1,p}(\Omega)$ with $p \geq 2$, together with the condition that the domain Ω be simply connected.

Regarding Q-tensor fields on manifolds (which we assume here to be compact, connected, without boundary), we observe that there exists no two-dimensional surface N and exponent $p \geq 2$ such that

$$Q \in W^{1,p}(N) \quad \Rightarrow \quad \text{Q is orientable.}$$

Indeed, by Proposition 4.1.1 the only surface which allows for the existence of a unit vector field with regularity at least $W^{1,2}$ is the torus, which is not simply connected, and on which simple examples of smooth nonorientable line fields can easily be constructed (see Fig. 4.2).

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Résumé

Dans cette thèse, nous nous intéressons aux cristaux liquides nématiques, qui sont une phase de la matière intermédiaire entre les liquides et les solides cristallins ; en particulier, les molécules peuvent se déplacer librement, mais elles tendent à s'orienter localement dans une direction commune. Ces états sont caractérisés par la présence de défauts ponctuels ou de ligne. L'objectif principal de cette thèse est d'apporter une contribution à l'étude mathématique des défauts, dans le cadre de la théorie variationnelle de Landau-de Gennes.

Dans le premier chapitre, nous nous intéressons aux minimiseurs de l'énergie dans des domaines bornés et réguliers de dimension deux. Nous nous intéressons au comportement asymptotique lorsque la constante élastique du matériau tend vers zéro. Nous montrons que les minimiseurs convergent vers une application localement harmonique, avec un nombre fini de singularités ponctuelles. Au voisinage de celles-ci, les minimiseurs sont biaxes, c'est-à-dire, deux directions d'alignement local sont présentes en tout point.

Le deuxième chapitre est consacré à l'analyse asymptotique des minimiseurs en dimension trois, en supposant l'énergie majorée par le logarithme de la constante élastique. Comme dans le cas bidimensionnel, nous obtenons un résultat de compacité des minimiseurs, mais cette fois l'application limite peut présenter à la fois des singularités ponctuelles et de ligne. Nous donnons aussi des conditions suffisantes pour que l'hypothèse sur l'énergie évoquée précédemment soit satisfaite.

Le troisième chapitre porte sur l'existence de minimiseurs à symétrie radiale dans une couronne en dimension trois. Nous montrons que, si la largeur de la couronne est petite ou la température est suffisamment basse, alors il existe un unique minimiseur, qui est à symétrie radiale, pour l'énergie de landau-de Gennes. Enfin, dans le dernier chapitre nous présentons une obstruction topologique à l'existence de champs de vecteurs unitaires de faible régularité, sur des variétés compactes à bord. Ce résultat peut être considéré comme une étape préliminaire à l'étude de certains modèles variationnels pour les films nématiques sur une surface.

Mots-clés. Landau-de Gennes, Q-tenseurs, uniaxialité et biaxialité, analyse asymptotique, singularités topologiques, défauts de ligne, ensembles rectifiables, solutions à symétrie radiale, hérisson radial, indice d'un champ de vecteurs, formule de Poincaré-Hopf-Morse, fonctions VMO (« Vanishing Mean Oscillation »).

Abstract

In this thesis we consider the Landau-de Gennes variational model for nematic liquid crystals. Nematic liquid crystals are an intermediate phase of matter, which shares properties both with liquids and crystalline solids. They are composed of molecules which can flow freely, but tend to align locally along some preferred directions. Nematic phases exhibit defects, which can occur at isolated points or along lines, and are one of their mean features. This thesis mainly aims at discussing some results towards the mathematical understanding of defects and their generation, within the framework of the Landau-de Gennes theory.

In the first chapter, we study minimizers of the energy functional in a bounded, smooth domain in dimension two. We are interested in their asymptotic behaviour as the elastic constant tends to zero. We show that minimizers converge to a locally minimizing harmonic map, with a finite number of point singularities. Moreover, minimizers are biaxial in the core of defects. Biaxiality means that more than one preferred direction of molecular alignment exists at a given point.

Chapter two deals with the asymptotic analysis of minimizers in dimension three. We assume that the energy is comparable to the logarithm of the elastic constant and prove a compactness result, as in the two-dimensional case. However, the limiting map is now allowed to have line singularities as well as point singularities. We also provide sufficient conditions for the logarithmic energy estimate to be satisfied.

In the third chapter, we study the existence of radially symmetric minimizers on spherical shells, in dimension three. We prove that, if the shell width is small enough or the temperature is low enough, then there exists a unique minimizer for the Landau-de gennes energy, which is radially symmetric. Finally, in chapter four, we discuss a topological obstruction to the existence of unit vector fields of low regularity on a compact manifold with boundary. This result can be understood as a first step in the analysis of some variational models for a surface coated with a thin nematic film.

Keywords. Landau-de Gennes, Q-tensors, uniaxial and biaxial tensors, asymptotic analysis, topological singularities, line defects, rectifiable sets, radially symmetric solutions, radial-hedgehog, index of a vector field, Poincaré-Hopf-Morse formula, functions of Vanishing Mean Oscillation.